LES of temporally evolving mixing layers by high-order filter schemes

By A. Hadjadj, H. C. Yee and B. Sjögreen

1. Motivation and objective

Over the past decade, the use of computational fluid dynamics (CFD) in engineering science has increased, not only for fundamental understanding of complex compressible turbulent physics, but also for the development and design of industrial devices. Owing to the recent progress in petascale computing, in tandem with advances in algorithm development for accurate direct numerical simulations (DNS) and large eddy simulations (LES) of shock-free compressible turbulence and turbulence with strong shocks, this type of DNS and LES computation has gradually been able to tackle more complex flows physics. Advances in flow visualization tools have paved the way to extracting valuable information from the computed results containing hundreds of terabyte of data. Examples include flows through internal propulsive nozzles with shock-wave propagation or sound emission from supersonic jets, and mixing and shock/boundary layer interactions.

Efficient and accurate DNS and LES simulations of the aforementioned flow physics, especially shock-wave/boundary layer interactions (SWBLI) for supersonic and hypersonic turbulence flows, are computationally very challenging due to the wide range of temporal and spatial length scales. For turbulent flows, the only known route to general high-fidelity flow simulations is through fully resolving all scales. The absence of scale separation makes it very difficult to take mathematical short cuts. State-of-the-art numerical methods for simulation of supersonic and hypersonic flows are designed to be robust enough to handle strong shock waves. However, these methods are not accurate enough to resolve a wide range of turbulent scales without additional improvement. In terms of turbulence modeling, there has been considerable progress in the development and usage of large eddy simulation (LES) for the simulation of turbulent flows in the past few decades. While a substantial amount of research has been carried out into modeling for the LES of incompressible flows, applications to compressible flows have been significantly fewer, due to the increased complexity introduced by the need to resolve a total energy equation, which introduces extra unclosed terms in addition to the subgrid-scale stresses that must be modeled in incompressible flows.

For the current investigation, the high-order nonlinear filter schemes with a pre- and postprocessing step are selected due to the efficiency, accuracy and highly parallelizable nature of the construction (Yee & Sjogreen 2009). Studies in Yee & Sjogreen (2009) and Yee et al. (2010) indicate that for turbulence with shock problems, an eighth-order spatial base scheme in conjunction with a dissipative portion of WENO7 (WENO7fi) is more accurate than its fourth- and sixth-order counterparts. Studies found that employing entropy splitting (Yee et al. 2000; Sjogreen & Yee 2009; Honein & Moin 2004) of the inviscid flux derivative can stabilize the central base scheme for smooth flows. In addition, this splitting is the most accurate among the aforementioned splitting methods. Indirectly, less numerical dissipation is needed when the split form is used. Unfortunately, entropy splitting is not suitable for problems with moderate and strong shocks as the split form
is not conservative. Due to the mixture of shock-free turbulence and turbulence with shocklets, for all of the computations shown later, the Ducros et al. (2000) splitting is employed since a conservative splitting is more appropriate.

In this paper we report recent progress in the development and validation of LES computations of compressible turbulent mixing layers using high-order numerical schemes. The current research is motivated by the long-term overarching goal of developing numerical tools for reliable predictive capability of complex turbulent flows, especially for problems including compressibility, heat transfer and real gas effects that interact with instabilities, shocks and turbulence.

2. LES of temporally evolving compressible mixing layers

LES of temporally evolving mixing layers (TML) between two streams moving with opposite velocities is considered, with $U_1 = -U_2 = \Delta U/2$. The three main characteristics of compressible mixing layers are: 1) the self-similarity property, which is characterized by linear growth of the layer as well as the mean velocities and turbulent statistics being independent of the downstream distance normalized by appropriate length and velocity scales; 2) the compressibility effects through turbulence damping and decrease of the mixing-layer growth rate for high convective Mach numbers; and 3) the presence of a large-scale structure with shocklets. These organized structures play an important role in the dynamics of the mixing layer, its spreading and energy transport. The objective of the current investigation is to verify that the numerical methods used in this study are capable of dealing with the three key points cited above. An other objective is to perform and validate a well-resolved spatial large-eddy simulation to obtain accurate and reliable data at higher Mach and Reynolds numbers.

2.1. Problem setup

The configuration of the temporally evolving mixing layer is shown in Figure 1. Five test cases (denoted LES-C_i, i = 1, ..., 5) are carried out with different convective Mach numbers ranging from the incompressible case $M_c = 0.1$ up to the supersonic one $M_c = 1.5$. The later corresponds to a highly compressible mixing layer, whereas the first two cases, $M_c = 0.1$ and $M_c = 0.3$, can be considered as quasi-incompressible and are used to compare with the experimental results of incompressible shear layer. All of the simulations described below are performed at an initial Reynolds number, $Re_\omega_0$, based on the mean velocity difference $\Delta U$, the average viscosity of the free streams and the vorticity thickness $\delta_\omega_0$ of 800 with $\delta_\omega_0 = 4 \delta_\phi$, where $\delta_\omega = \Delta U/(\partial u/\partial y)_{max}$ is the vorticity thickness of the shear layer, and $\delta_\phi$ is the momentum thickness given by Eq. 2.2. $Re_\omega$ reaches values as large as $3 \times 10^5$ at the end of the simulation, which is one order of magnitude higher than the similar DNS and LES computations reported in the literature (Pantano & Sarkar 2002; Mahle et al. 2007; Foysi & Sarkar 2010). Table 1 summarizes the details of flow parameters for both LES and previous DNS data in the literature. The mean flow is initialized with a tangent hyperbolic profile for the streamwise velocity, $u(y) = \frac{1}{2} \Delta U \tanh \left[ y/(2 \delta_\phi) \right]$, while the two other velocity components are set to zero. In addition to these mean values, three-dimensional turbulent fluctuations $(u', v', w')$ are imposed, while initial pressure and density are set constant. Since the simulation is temporal, the initial perturbations are added only once to the velocity field using a digital filter technique (Klein et al. 2003). This procedure utilizes the prescribed Reynolds stress tensor and length scales of the problem concerned to generate the corresponding fluctuating velocity field, taking into account the nature of autocorrelation function for the
prevailing turbulence. The length scales are chosen as \( \delta_{u_0} \) in each direction. The Reynolds stress tensor is assumed to have a Gaussian shape with amplitudes taken similar to the experimental peak intensities available for the incompressible mixing layer (Bell & Mehta 1990).

Periodic boundary conditions are enforced in the streamwise \((x)\) and spanwise \((z)\) directions, while non-reflecting conditions are applied in both top and bottom boundaries \((y)\) direction). The use of a periodic boundary condition in the \(x\) direction corresponds to the temporal formulation of mixing layer evolution, which is supposed to evolve only in time as it spreads in \(y\).

### 2.2. Mesh requirements

Similarly to Foysi & Sarkar (2010), a large computational domain of lengths \(L_x \times L_y \times L_z = 1200 \delta_{u_0} \times 370 \delta_{u_0} \times 270 \delta_{u_0}\) is used with the corresponding mesh points \(N_x \times N_y \times N_z = 512 \times 211 \times 131\). The same grid system uniformly spaced in the \(x\) and \(z\) directions and stretched in the \(y\) direction is employed for all cases considered. The High Resolution (HR) grid used in this study contains an order of magnitude fewer cells than that of the DNS of Pantano & Sarkar (2002) compared to the domain length. The emphasis of the HR simulation is to produce an LES solution that predicts the trends of the DNS as well as experimental data for both quasi-incompressible and highly-compressible mixing layers. To ensure that the computational domain in the \(x\) and \(z\) directions is sufficiently wide, the two-point correlation functions are analyzed,

\[
R_{\phi\phi}(r) = \sum_{k=1}^{N-k_r} \phi_k \phi_{k+k_r}, \quad k_r = 0, 1, ..., N - 1,
\]

where \(r = k_r \Delta\), \(N\) is half of the number of grid points in the homogeneous directions with grid size \(\Delta\) and \(\phi\) represents the fluctuations of flow variables.

The computed two-point autocorrelation coefficients \(R_{\phi\phi}(r)/R_{\phi\phi}(0)\) (pressure as well as velocity components) in the homogeneous directions \((x\) and \(z)\) are reported in Figure 2 as a function of the distance in the stream- and spanwise coordinates at the middle of the mixing layer \((L_y/2)\) and at \(\tau = 2500\). The two part of the figure show that the flow variables are sufficiently decorrelated over distances \(L_x/2\) and \(L_z/2\), thus ensuring that the streamwise as well as the spanwise extents of the computational domain are sufficient so as to not inhibit turbulence dynamics. Also, the length in \(y\) direction is selected to be large enough for the flow to achieve a fully developed state. In terms of turbulent length scales, the Kolmogorov length scale \(\eta\) and an average (isotropic)Taylor micro-scale \(\lambda\) are
Table 1. Flow parameters and turbulent length scales during the quasi-self-similar stage, corresponding to $\tau = 600$ for LES-C1/C2 and $\tau = 2500$ for LES-C3,...,C5).

<table>
<thead>
<tr>
<th>Case</th>
<th>$M_c$</th>
<th>$Re_{\omega_0}$</th>
<th>$L_x/\Lambda_x$</th>
<th>$L_z/\Lambda_z$</th>
<th>$\Delta y_{\min}/\lambda$</th>
<th>$\Delta y_{\min}/\eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNS Rogers &amp; Moser (1994)</td>
<td>0</td>
<td>800</td>
<td>-</td>
<td>-</td>
<td>&gt; 1</td>
<td>$\approx$ 1</td>
</tr>
<tr>
<td>DNS Pantano &amp; Sarkar (2002)</td>
<td>0.3</td>
<td>640</td>
<td>20.4</td>
<td>15.3</td>
<td>0.64</td>
<td>49.3</td>
</tr>
<tr>
<td>LES-C1</td>
<td>0.1</td>
<td>800</td>
<td>30.2</td>
<td>15.1</td>
<td>0.64</td>
<td>49.5</td>
</tr>
<tr>
<td>LES-C2</td>
<td>0.3</td>
<td>800</td>
<td>30.2</td>
<td>15.1</td>
<td>0.65</td>
<td>49.5</td>
</tr>
<tr>
<td>LES-C3</td>
<td>0.8</td>
<td>800</td>
<td>12.1</td>
<td>11.0</td>
<td>0.74</td>
<td>50.1</td>
</tr>
<tr>
<td>LES-C4</td>
<td>1.0</td>
<td>800</td>
<td>12.0</td>
<td>11.4</td>
<td>0.67</td>
<td>53.7</td>
</tr>
<tr>
<td>LES-C5</td>
<td>1.5</td>
<td>800</td>
<td>12.0</td>
<td>10.2</td>
<td>0.82</td>
<td>55.2</td>
</tr>
</tbody>
</table>

Defined as $\eta = (\nu^3/\varepsilon)^{1/4}$, $\lambda = \sqrt{15 \nu k/\varepsilon}$, where $k = \frac{1}{2}(u'^2 + v'^2 + w'^2)$ is the turbulent kinetic energy. The computed integral length scales ($\Lambda_x, \Lambda_z$) and the Kolmogorov scale are also given in Table 1 for further comparison. In our case the integral scales are given by

$$\Lambda_x = \int_0^{L_x/2} \frac{\langle u_i(x_i, t) u_i(x_i + p, t) \rangle}{\langle u_i^2 \rangle} dp,$$

$$\Lambda_z = \int_0^{L_z/2} \frac{\langle u_i(x_i, t) u_i(x_i + p, t) \rangle}{\langle u_i^2 \rangle} dp,$$

and $p$ is the distance between two points in the flow. The integral length scale is important in characterizing the structure of turbulence. It is a measure of the longest correlation distance between the flow velocity (or vorticity, etc.) at two points in the flow field. Recent work concludes that a reasonable lower limit on the domain must be at least six times larger than the integral length (O’Neill et al. 2004). This recommendation is consistent with the data shown in Table 1, where the spatial domain is between ten and thirty times larger than the integral length. Also, it is evident from Table 1 that the integral lengths are sufficiently small compared to the computational domain and the grid resolution is adequate to resolve the large scales of turbulence.

Owing to the high computational cost of the simulations, the numerical code is fully parallelized running on up to 600 processors. In total, the present simulation required 2000 CPU hours each on modern SGI IC, Pleiades and Columbia supercomputers of NASA NASA-Ames.

2.3. Mean flow and turbulent statistics

LES computations are carried out up to dimensionless time $\tau = t \Delta U/\delta \theta_0 \approx 3000$ for the higher convective Mach number cases and $\tau \approx 1200$ for the quasi-incompressible cases. In order to compare the LES results with experimental data, the time-averaged flow quantities $\langle \overline{\varphi} \rangle$ and $\langle \overline{\varphi} \rangle$ are extracted from the flow field during the self-similar time period ($600 < \tau < 1000$ for LES-C1 and LES-C2 and $2000 < \tau < 2800$ for LES-C3, LES-C4 and LES-C5). Note that throughout this paper only resolved quantities are considered; subgrid-scale contributions are not added onto, e.g., the turbulent stresses. To validate the low-Mach-number LES case, previous DNS studies of the incompressible shear layer, including Rogers & Moser (1994), Pantano & Sarkar (2002), as well as experimental studies by Bell & Mehta (1990) and Spencer & Jones (1971), are used. Further experimental results on the compressible shear layer (Papamoschou & Roshko 1988; Elliott & Samimy
LES of temporally evolving mixing layers

Figure 2. Streamwise and spanwise autocorrelation functions for LES-C5 at $\tau = 2500$.

Figure 3. (left) Time evolution of normalized momentum thickness for LES-C2 compared to the DNS of Pantano & Sarkar (2002) for $M_c = 0.3$. (right) Comparison of normalized mean streamwise velocity for LES-C1 and LES-C2.

1990; Barre et al. 1997; Chambres et al. 1998) and DNS results obtained by Pantano & Sarkar (2002) are used to compare with the high-Mach-number simulations.

As recommended by Rogers & Moser (1994), the momentum thickness $\delta_\theta$ is used for self-similar scaling rather than the vorticity thickness $\delta_\omega$, because it is less sensitive to statistical noise as it is an integral quantity evolving smoothly in time, whereas $\delta_\omega$ is obtained from the derivative of the mean velocity and may exhibit oscillations during flow evolution. Therefore, the time evolution of the momentum thickness of the flow calculated using the definition

$$\delta_\theta = \int_{-\infty}^{+\infty} \frac{\bar{\rho}}{\rho_{ref}} \left( \frac{1}{4} - \frac{\bar{u}^2}{\Delta U^2} \right) dy \quad (2.2)$$

is shown in Figure 3. Excellent agreement with the DNS simulation is obtained and the linear slope is recovered after a short transient, showing the self-similar state of the mixing layer. The growth rate $d(\delta_\theta/\delta_\theta_0)/d\tau$ (slope of the linear curve fit) for this case is found to be 0.016. The ratio of vorticity thickness to momentum thickness ($D_\omega = \delta_\omega/\delta_\theta \simeq 4.5$) with $Re_\omega = 603391$ at $\tau_{max}$ $\simeq 1200$. This is in excellent agreement with the DNS growth rate of the quasi-incompressible case with $M_c = 0.3$ of Pantano & Sarkar (2002). Note that in Eq. 2.2, $\langle \cdot \rangle_{ref}$ represents the reference state which is the arithmetic mean of the free streams 1 and 2.
Table 2. Comparison of peak turbulent intensities of incompressible mixing layer

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>$M_c$</td>
<td>0</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$\sqrt{\langle R_{11} \rangle} / \Delta U$</td>
<td>0.18</td>
<td>0.155</td>
<td>0.17</td>
</tr>
<tr>
<td>$\sqrt{\langle R_{22} \rangle} / \Delta U$</td>
<td>0.14</td>
<td>0.134</td>
<td>0.134</td>
</tr>
<tr>
<td>$\sqrt{\langle R_{33} \rangle} / \Delta U$</td>
<td>0.146</td>
<td>0.143</td>
<td>0.143</td>
</tr>
<tr>
<td>$\sqrt{-\langle R_{12} \rangle} / \Delta U$</td>
<td>0.10</td>
<td>0.103</td>
<td>0.106</td>
</tr>
<tr>
<td>$\sqrt{\langle R_{22} \rangle / \langle R_{11} \rangle}$</td>
<td>0.777</td>
<td>0.788</td>
<td>0.788</td>
</tr>
<tr>
<td>$\sqrt{-\langle R_{12} \rangle / \langle R_{11} \rangle}$</td>
<td>0.555</td>
<td>0.606</td>
<td>0.623</td>
</tr>
</tbody>
</table>

The normalized mean streamwise velocity for LES-C1 and LES-C2 are presented in Figure 3. It can be seen that the two LES profiles collapse together and are in excellent agreement with both DNS (Pantano & Sarkar 2002) and experimental results (Bell & Mehta 1990; Spencer & Jones 1971).

Further validation of the present LES is achieved through the comparison of turbulent intensities in the self-similar region (calculated by averaging over profiles plotted in similarity coordinates) seen in Figure 4, where different components of the normalized Reynolds stress tensor, $\sqrt{|R_{ij}|} / \Delta U$ ($R_{ij} = \rho u'_i u'_j / \bar{p}$), are compared to DNS and experimental data. Table 2 summarizes the comparison of peak turbulent intensities, as well as the anisotropic deviation on the centerline of the layer. It is evident that very good agreement between the present LES and previous results is obtained for this measure of anisotropy. Both LES-C1 and LES-C2 give almost the same results, probably because both are in incompressible (or weakly-compressible) regimes.

2.4. Compressibility effects

Apart from studying the self-similarity property in the mixing layer, the effects of convective Mach number are also investigated using LES. Figure 5 shows the time evolution of momentum thickness for various convective Mach numbers. After a relatively long time ($\tau > 2000$ compared to the incompressible one), corresponding to the initial transient, the mixing layer grows quasi-linearly with spread rates of $d(\delta / \delta_0) / d\tau = 0.0165, 0.0101, 0.0084$ and $0.0075$ for cases LES-C2, LES-C3, LES-C4 and LES-C5, respectively.

In compressible mixing layers, all of the assessments of compressibility effects can be related to the convective Mach number, $M_c$, through the compressibility factor, $\Phi = (d\delta / d\tau)_c / (d\delta / d\tau)_i$, which is the ratio of the compressible growth rate to the incompressible growth rate at the same velocity and temperature ratios. The calculated compressibility factor is significantly less than the incompressible counterpart, the ratio of the two being less than 0.43 for $M_c > 1$. This is consistent with previous findings on the effects of compressibility on mixing-layer growth rate such as the nonlinear regression fit of Barone et al. (2006) and Oberkampf & Barone (2006) plotted in Figure 5. This plot shows the ratio of compressible mixing-layer growth to incompressible mixing-layer
growth rate as a function of $M_c$, and data from different experiment and previous DNS have been included for comparison. The two higher compressibility cases have growth rates which agree well with previously published data. As already pointed out by Papamoschou (1993), the growth-rate reduction starts at subsonic values of $M_c$ and is evidently completed before $M_c$ becomes supersonic (Figure 5). This implies that compressibility takes effect before any shock or expansion waves appear in the flow, in the convective frame of reference. The data in this figure exhibit significant scattering that is partly attributed to the different experimental conditions. Concerning the 90% confidence interval, it is seen that the largest uncertainty in the experimental data occurs for large $M_c$. As pointed out by Barone et al. (2006), future investigations should be conducted at higher convective Mach numbers to better determine the asymptotic value of $\Phi$. Also, the simulations show that the turbulence intensity decreases with increasing convective Mach number (results not shown for space considerations). The decreased level of energy is responsible for the reduction of the mixing thickness growth rate as already pointed out by Samimy et al. (1992); Vreman et al. (1996) and many other LES and DNS studies (Pantano & Sarkar 2002; Foysi & Sarkar 2010; Sandham & Reynolds 1989).

2.5. Flow structures and shocklets

The invariant of velocity gradient tensor $Q$ and the corresponding normalized form $\Lambda$ are defined by

$$Q = \frac{1}{2} [\Omega_{ij} \Omega_{ij} - S_{ij} S_{ij}], \quad \Lambda = \frac{[\Omega_{ij} \Omega_{ij} - S_{ij} S_{ij}]}{[\Omega_{ij} \Omega_{ij} + S_{ij} S_{ij}]}.$$  

(2.3)
Figure 5. (left) Time evolution of normalized momentum thickness for LES at different convective Mach numbers (with higher $M_c$ corresponding to lower curves). (right) Compressibility factor as a function of the convective Mach number from different experimental mixing-layer studies selected by Barone et al. (2006): (a) Bogdanoff (1983); Papamoschou & Roshko (1988); (b) Chinzei et al. (1986); (c) Samimy & Elliot (1990); Samimy et al. (1992); Elliott & Samimy (1990); — nonlinear regression curve from Barone et al. (2006) with $\Phi(M_c) = 1 - a_1 \left(1 - 1/(1 + a_2 M_c^{a_3})\right)$, $a_1 = 0.5537$, $a_2 = 31.79$, $a_3 = 8.426$.

where $S_{ij} = (u_{i,j} + u_{j,i})/2$, $\Omega_{ij} = (u_{i,j} - u_{j,i})/2$.

The iso-surfaces of $Q$ and $\Lambda$ are plotted for flow visualization of mixing layers. The positive values of $Q$ and $\Lambda$ represent the vortex dominated flow. Three-dimensional perspective views of iso-surfaces of $Q$ are presented in Figure 6 for LES-C2 in self-similar state. The 3D complex vortex tubes structures are clearly evident from these figures.

With regard to the highly compressible case, the complexity of three-dimensional flow structure leads to the difficulties in the identification of the shocklets. One good method to identify the location of a shock is to use a Schlieren-based technique to portray shocks and even more weak discontinuity in the fluid (see Hadjadj & Kudryavtsev 2005). Since in our case the initial density is uniform, we used the Schlieren technique based on the dilatation of the velocity field $\nabla u$ to highlight the eddy shocklets (see Figure 7). Note that shocklets start to appear at Mach number less than unity, i.e., in the lower part of the transsonic regime. As expected, for higher Mach numbers the shocklets become stronger and are preferentially organized in oblique waves (see Figure 7), corresponding to stationary inviscid shocks at a dominant propagation direction, $\theta$, and a nominal Mach number, $M_n = \Delta U/(2c)$, where $c$ is the speed of sound in the unperturbed region. From our computation, it can be seen that oblique structures start to occur at Mach numbers less than unit. These structures related to compression waves emanating from the shear layer and also the existence of other perturbing pressure disturbances lead to enhanced mixing through the creation of streamwise vortices.

3. Summary

This paper illustrates some recent progress in computations of compressible turbulence using high-order spatial schemes on an LES model for temporally evolving turbulent mixing layers. Results obtained including flow visualization, streamwise velocities, fluctuating velocities and Reynolds stresses agree well with experimental results. In particular, the current LES agree with the previous DNS of the mixing layer by Vreman et al. (1996) and Freund et al. (2000) that show decreased turbulence production with increasing $M_c$. The
Figure 6. Iso-surface of $Q = 0.01Q_{\text{max}}$ colored by density at $\tau = 1000$ and for LES-C2

The present study serves as a validation of the performance of the improved filter schemes of Yee & Sjogreen (2009) on a representative complex compressible turbulent flow consisting of a wide range of flow speeds.

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Figure 7. Instantaneous numerical Schlieren pictures at $\tau = 2000$ for LES-C5

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