LARGE EDDY SIMULATION OF
THREE DIMENSIONAL HIGH SPEED AERODYNAMIC FLOWS

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An unstructured grid Large Eddy Simulation (LES) methodology has been developed for compressible high speed flows. The filtered compressible Navier-Stokes equations are solved on an unstructured grid of tetrahedra. The inviscid fluxes are obtained from an exact locally one-dimensional Riemann solver using Godunov's method. The viscous fluxes are obtained using a discrete analog of Gauss' Theorem. The reconstruction is performed using a Least Squares technique. The temporal integration is a Runge-Kutta method. The algorithm is overall second order accurate in space and time. Four flowfields have been computed: supersonic flat plate boundary layer, supersonic compression corner, supersonic expansion-compression corner and subsonic square jet. The computed results show close agreement with experiment and Direct Numerical Simulation, and validate the unstructured grid LES methodology.
Abstract

An unstructured grid Large Eddy Simulation (LES) methodology has been developed for compressible high speed flows. The filtered compressible Navier-Stokes equations are solved on an unstructured grid of tetrahedra. The inviscid fluxes are obtained from an exact locally one-dimensional Riemann solver using Godunov's method. The viscous fluxes are obtained using a discrete analog of Gauss' Theorem. The reconstruction is performed using a Least Squares technique. The temporal integration is a Runge-Kutta method. The algorithm is overall second order accurate in space and time. Four flowfields have been computed: supersonic flat plate boundary layer, supersonic compression corner, supersonic expansion-compression corner and subsonic square jet. The computed results show close agreement with experiment and Direct Numerical Simulation, and validate the unstructured grid LES methodology.
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Introduction

The effective design of high speed aircraft and missiles depends critically upon accurate prediction of aerodynamic and aerothermodynamic performance which are strongly affected by flow turbulence under most flight conditions. From an engineering standpoint, the aircraft or missile aerodynamicist needs the capability for accurate prediction of the mean and rms fluctuating surface pressure ($p_w$ and $p'_w$) and surface heat transfer ($\bar{q}_w$ and $q'_w$), mean surface skin friction ($\bar{\tau}_w$), and locations of primary and secondary separation.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Satisfactory</th>
<th>Unsatisfactory</th>
<th>No capability shown</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_w$</td>
<td>✓</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>$p'_w$</td>
<td></td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>$\bar{q}_w$</td>
<td></td>
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<td>$q'_w$</td>
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<td></td>
<td>✓</td>
</tr>
<tr>
<td>Primary Separation</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Secondary Separation</td>
<td></td>
<td></td>
<td>✓</td>
</tr>
</tbody>
</table>

The current methodology for prediction of compressible turbulent flows is based on the Reynolds-averaged Navier-Stokes (RANS) equations (Knight 1993). This approach has yielded a hierarchy of turbulence models extending from zero-equation to full Reynolds Stress Equation models. While these models have generally been capable of predicting the engineering quantities of interest in weakly perturbed boundary layers, they have been unable to accurately predict the complex 3-D flows which are encountered in highly maneuvering, high angle-of-attack flight. Two recent extensive reviews have documented the capabilities and deficiencies of a wide range of RANS models for prediction of complex 3-D flows with shock wave-turbulent boundary layer interactions (Knight 1997, Knight and Degrez 1998). The results, summarized in Table 1, indicate that a significant number of critical engineering quantities are not capable of prediction by current RANS models. Therefore, more advanced turbulence models are needed which have the ability to simulate the complex physics of turbulence with greater generality.

Large Eddy Simulation (LES) is an alternative to RANS which may be capable of predicting more (or all) of the aerodynamic and aerothermodynamic quantities of engineering interest described above. In LES, the governing equations are spatially filtered on the scale of the numerical grid. The large, energy-containing eddies are directly computed. These eddies are strongly influenced by the physical geometry and configuration of the flow. Thus, the direct computation of the large eddies by LES, as opposed to the modeling of the large eddies by RANS, gives greater generality, in principle, to LES. The influence of the unresolved scales of motion is simulated using a subgrid-scale (SGS) model (Smagorinsky 1963, Lilly 1967, Deardorff 1970, Germano et al 1991, Piomelli et al 1991, Ghosal et al 1995) or by the inherent dissipation in the numerical scheme (Boris et al 1992, Oran and Boris 1993, Porter et al 1994, Grinstein 1996, Ansari and Strang 1996). Because the statistics of the small scale turbulence are expected to be more homogeneous and isotropic than those of the large scales, a general model of the small scales seems more plausible than a general model of the entire spectrum of turbulent motions.

LES has been shown to be both a useful research tool for understanding the physics of turbulence, and also a predictive method for flows of engineering interest. Recent compendia and reviews include Galperin and Orszag (1993), Mason (1994), Lesieur and Métais (1996) and Moin (1997).
Many models have been developed for the subgrid-scale stress tensor. These include the conventional Smagorinsky eddy viscosity model (Smagorinsky 1963, Lilly 1967, Deardorff 1970), the spectra eddy viscosity model of Kraichnan (1976), the dynamic SGS model of Germano et al (1991), the scale similarity model of Bardina et al (1980), and the localized dynamic SGS model of Ghosal et al (1995) and more recently of Menon and Kim (1996), and many others. Although most research has focused on incompressible turbulent flows, there has recently emerged a growing interest in applications of LES to compressible turbulent flows. Examples include Yoshizawa (1986), Speziale et al (1988), Moin et al (1991), Erlebacher et al (1992), Zang et al (1992), El-Hady et al (1994), Jansen (1997), Spyropoulos and Blaisdell (1996), and Haworth and Jansen (1996). Nearly all compressible LES has employed spectral methods or structured grids, with the exception of Jansen and Haworth.

Apart from the complexities of the flowfield, the complicated geometries of high speed vehicles is also a challenge. To enable treatment of complex geometries and also achieve high resolution of the flowfield dynamically, we employ an unstructured grid. There are two important advantages of unstructured grids. First, algorithms have been developed to facilitate automatic generation of unstructured grids for a complex geometries (see, for example, the discussion in Barth (1990, 1992). These grid generation methods can be substantially more efficient (in terms of user time) than some of the multi-block structured grid generation methods used. Second, local mesh refinement, either adaptive or fixed, can be performed much more readily for unstructured grids.

The report summarizes the research in Large Eddy Simulation of compressible turbulent flows using unstructured grids. Two methods for simulation of the subgrid scale stresses have been examined. The first method is the Monotone Integrated Large Eddy Simulation (MILES) technique. The second method is a hybrid technique combining MILES with a Smagorinsky eddy viscosity model for the subgrid scale stresses. These two methods, together with different algorithms for the inviscid fluxes and function reconstruction, have been evaluated for four turbulent flows: supersonic boundary layer, supersonic compression corner, supersonic expansion-compression corner and subsonic square jet. The results are in overall good agreement with the experiment and Direct Numerical Simulation (DNS), thereby validating the accuracy of the methodology.

**Governing Equations**

The governing equations are the three-dimensional filtered Navier-Stokes equations. For a function \( f \), its filtered form \( \tilde{f} \) is

\[
\tilde{f} = \frac{1}{V} \int_V G f \, dV
\]

where \( G \) is the filtering function, and its Favre-averaged form \( \bar{f} \) is

\[
\bar{f} = \frac{\rho \tilde{f}}{\bar{\rho}}
\]

where \( \rho \) is the density. From the Navier-Stokes equations for the instantaneous flow variables density \( (\rho) \), velocity in the \( i \)th coordinate direction \( (u_i) \), pressure \( (p) \) and temperature \( (T) \), Favre-averaging and spatial filtering yield the filtered Navier-Stokes equations (here written using the Einstein summation notation where repeated indices denote summation)

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \tilde{u}_k}{\partial x_k} = 0
\]

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{u}_k}{\partial x_k} = \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k}
\]
\[ \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_k} (\bar{p} \bar{u}_k) = \frac{\partial Q_k}{\partial x_k} + \frac{\partial}{\partial x_k} (T_{ik} \bar{u}_i) \]

where

\[ T_{ik} = \tau_{ik} + \bar{\sigma}_{ik} \]
\[ \tau_{ik} = -\bar{p} (\bar{u}_i \bar{u}_k - \bar{u}_k \bar{u}_i) \]
\[ \bar{\sigma}_{ik} = \mu(T) \left( -\frac{2}{3} \frac{\partial \bar{u}_j}{\partial x_j} \delta_{ik} + \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial \bar{u}_k}{\partial x_i} \right) \]
\[ Q_k = Q_k + \bar{q}_k \]
\[ Q_k = -\bar{\rho}c_p (T \bar{u}_k - \bar{T} \bar{u}_k) \]
\[ \bar{q}_k = k(T) \frac{\partial \bar{T}}{\partial x_k} \]
\[ \bar{\rho} \bar{e} = \bar{\rho}c_v \bar{T} + \frac{1}{2} \bar{\rho} \bar{u}_i \bar{u}_i + \bar{\rho} \bar{k} \]
\[ \bar{\rho} \bar{k} = \frac{1}{2} (\bar{\rho} \bar{u}_i \bar{u}_i - \bar{\rho} \bar{u}_j \bar{u}_j) = -\frac{1}{2} \tau_{ii} \]

Two different Sub-Grid-Scale (SGS) models are employed. The first model is Monotone Integrated Large Eddy Simulation (MILES) wherein the numerical algorithm itself provides the requisite dissipation associated with the subgrid scale motions. The second model is the classical constant-coefficient Smagorinsky method.

\[ \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \]
\[ \tau_{ij} = 2C_R \tilde{\rho} \Delta^2 \sqrt{\tilde{S}_{mn} \tilde{S}_{mn}} \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) \]
\[ Q_j = \bar{\rho}c_p C_R \frac{\Delta^2 \sqrt{\tilde{S}_{mn} \tilde{S}_{mn}}}{Pr} \frac{\partial \bar{T}}{\partial x_j} \]

where \( C_R = 0.00423 \) and \( \Delta \) is the length scale which is related to the local grid size. For boundary layer flows, \( \Delta \) is multiplied by the Van Driest damping factor

\[ D = 1 - e^{-n^+ / A} \]

where \( A = 26, n^+ = n u_r / \nu_w \) is the normal distance to the (nearest) solid boundary normalized by the viscous length scale \( \nu_w / u_r \) where \( \nu_w \) is the kinematic viscosity evaluated at the wall and \( U_r \) is the local friction velocity.

We simplify the notation by hereafter dropping the tilde \( \tilde{} \) and overbar \( \bar{} \). The flow variables are nondimensionalized using the reference density \( \rho_\infty \), velocity \( U_\infty \), static temperature \( T_\infty \) and length scale \( L \), with Mach number \( M_\infty = U_\infty / \sqrt{\gamma R T_\infty} \). The governing equations are therefore

\[ \frac{\partial \bar{p}}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0 \]
\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_k}{\partial x_k} = -\frac{\partial p}{\partial x_i} + \frac{\partial T_{ik}}{\partial x_k} \\
\frac{\partial \rho e}{\partial t} + \frac{\partial}{\partial x_k} (\rho e + p) u_k = \frac{\partial}{\partial x_k} (Q_k + T_{ik} u_i) \\
\rho = \frac{\rho T}{\gamma M^2_{\infty}}
\]

**Numerical Algorithm**

The governing equations are expressed in finite volume form for a control volume \( V \) with surface \( \partial V \)

\[
\frac{d}{dt} \int_V Q dV + \int_{\partial V} (F_i + G_j + H_k) \cdot \hat{n} dA = 0
\]

where \( Q \) is the vector of dependent variables

\[
Q = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho e
\end{pmatrix}
\]

and the flux vectors are

\[
F = \begin{pmatrix}
\rho u \\
\rho u^2 + p - T_{xx} \\
\rho u v - T_{xy} \\
\rho u w - T_{xz} \\
(\rho e + p) u - Q_x - \beta_x
\end{pmatrix}, \quad G = \begin{pmatrix}
\rho v \\
\rho u v - T_{xy} \\
\rho v^2 + p - T_{yy} \\
\rho v w - T_{yz} \\
(\rho e + p) v - Q_y - \beta_y
\end{pmatrix}, \quad H = \begin{pmatrix}
\rho w \\
\rho u w - T_{xz} \\
\rho v w - T_{yz} \\
\rho w^2 + p - T_{zz} \\
(\rho e + p) w - Q_z - \beta_z
\end{pmatrix}
\]

with

\[
\beta_x = T_{xx} u + T_{xy} v + T_{xz} w \\
\beta_y = T_{xy} u + T_{yy} v + T_{yz} w \\
\beta_z = T_{xz} u + T_{yz} v + T_{zz} w
\]

An unstructured grid of tetrahedra is employed, with a cell-centered storage architecture. The cell-averaged values, stored at the centroid of each tetrahedron of volume \( V_i \) are

\[
Q_i = \frac{1}{V_i} \int_{V_i} Q dV
\]

The inviscid fluxes are computed using Godunov's method which is an exact one-dimensional Riemann solver (Gottlieb and Groth 1988) applied normal to each face. The inviscid flux computations require the values of each variable on either side of the cell faces. These values are obtained from the cell-averaged values by second-order or third-order function reconstruction using the Least Squares
method of Ollivier-Gooch (Ollivier-Gooch 1997). The second-order function reconstruction method of Frink (1994) was employed in some of the earlier LES studies, but was found inferior to the method of Ollivier-Gooch (Okong'o and Knight 1998). More details on the reconstruction schemes are given in Okong'o and Knight (1998).

The viscous fluxes and heat transfer are computed by application of Gauss' theorem to the control volume whose vertices are the centroids of the cells which share each node. The second-order accurate scheme (in 2-D) is given by Knight (1994) and the extension to 3-D is straightforward.

**Parallelization**

The code is parallelized using domain decomposition and Message Passing Interface (MPI). Domain decomposition is performed in a pre-processing step. The domain is decomposed in a single direction with equal number of tetrahedra in each domain. A halo of cells is added in each domain to provide data on the adjacent domain, and the halo cell data is updated at every subiterate of the time integration. An example is shown in Fig. 1 for the LES of decay of isotropic turbulence. The numerical algorithm achieves excellent parallel performance. For example, the speed-up on four processors of the SGI Power Onyx with R-10000 processors is 3.7 for 93% efficiency (Knight et al 1998).

![Example of domain decomposition](image)

**Results**

Four different configurations have been examined: supersonic flat plate boundary layer, supersonic compression corner, expansion-compression corner and subsonic square jet.

1 Supersonic Flat Plate Turbulent Boundary Layer

The adiabatic and isothermal flat plate turbulent boundary layers at Mach 3 and Mach 4 at Reynolds number \( Re_5 = 2 \times 10^4 \) (based on the incoming boundary layer thickness \( \delta \) ) have been computed. The Reynolds number based on the momentum thickness \( \delta_2 \) and wall viscosity \( \mu_w \) is \( Re_{\delta_2} = 600 \). The Reynolds number is sufficiently high to achieve turbulent flow.

The inflow conditions are obtained using a compressible extension of the method of Lund *et al* (1998). The simulation generates its own inflow conditions through a sequence of operations where the velocity field at a downstream station is rescaled and reintroduced at the inflow boundary (Fig. 2). Defining \( x, y \) and \( z \) to denote the streamwise, transverse and spanwise directions, respectively, the size of the computational domain is \( L_x = 14.8\delta \), \( L_y = 3.4\delta \) and \( L_z = 2.0\delta \). The spanwise width \( L_z \) is approximately three times the experimental spanwise streak spacing (assuming the compressible turbulent boundary layer streaks scale in accordance with incompressible experimental results). The streamwise length \( L_x \) is approximately three times the mean experimen-
tal streamwise streak size. The height $L_y$ is based on the requirement that acoustic disturbances originating at the upper boundary do not interact with the boundary layer on the lower wall.

The reference quantities for non-dimensionalization are the incoming boundary layer thickness $\delta$, velocity $U_\infty$, density $\rho_\infty$, static temperature $T_\infty$ and molecular viscosity $\mu_\infty$ (where the subscript $\infty$ denotes the freestream condition). The grid resolution near the wall is dependent on $\Delta x^+$, $\Delta y^+$ and $\Delta z^+$, where $\Delta x^+ = \Delta x/\eta$, $\Delta y^+ = \Delta y/\eta$ and $\Delta z^+ = \Delta z/\eta$. The inner length scale is $\eta = \nu_w/u_\tau$, where $\nu_w$ is the kinematic viscosity at the wall, $u_\tau = \sqrt{\tau_w/\rho_w}$ is the friction velocity, $\tau_w$ is the wall shear stress and $\rho_w$ is the density at the wall. Before we proceed with the discussion about the grid resolution, we first describe how to obtain $\eta$.

The theoretical value of the friction velocity $u_\tau$ for a supersonic flat plate boundary is obtained from the combined Law of the Wall and Wake evaluated at $y = \delta$

$$\frac{U_{VD}}{u_\tau} = \frac{1}{\kappa} \ln(y + \frac{u_\tau}{\nu_w} + C + \frac{2\Pi}{\kappa} \sin^2 \left( \frac{\pi}{2} \frac{y}{\delta} \right)$$  \hspace{1cm} (1)

where

$$U_{VD} = \frac{U_\infty}{A} \left[ \sin^{-1} \left( \frac{2A^2 (\frac{U}{U_\infty}) - B}{\sqrt{B^2 + 4A^2}} \right) + \sin^{-1} \left( \frac{B}{\sqrt{B^2 + 4A^2}} \right) \right]$$  \hspace{1cm} (2)

$$\nu_w = \nu_\infty \left( \frac{T_w}{T_\infty} \right)^{1+\omega}$$

$$A = \left( \frac{\gamma - 1}{2} Pr_{tm} M_\infty^2 \frac{T_\infty}{T_w} \right)^{1/2}$$

$$B = \frac{T_{aw}}{T_w} - 1$$

$$T_{aw} = T_\infty \left[ 1 + \frac{(\gamma - 1)}{2} Pr_{tm} M_\infty^2 \right]$$

where $\kappa = 0.4$ is von Karman’s constant, $C = 5.1$, the wake parameter $\Pi$ is 0.12 at $Re_\delta = 2 \times 10^4$, the exponent $\omega$ is 0.76, the mean turbulent Prandtl number $Pr_{tm}$ is 0.89 and the ratio of specific
heats $\gamma$ is 1.4. The wall temperature $T_w$ is fixed at 10% above the theoretical adiabatic temperature $T_{aw}$ for the isothermal boundary. In the computation, $u_r$ and $\nu_w$ are obtained from $u_r = \sqrt{\tau_w / \rho_w}$ and $\nu_w = \nu_{\infty}(T_{aw})^{1+\omega}$, respectively.

The variation of Mach number and the different temperature boundary condition have effect on $\eta$, therefore on $\Delta x^+, \Delta y^+$ and $\Delta z^+$. At the same Mach number, the wall temperature for the isothermal case is 10% higher than that for the adiabatic case, leading to the larger $\eta$ and the smaller $\Delta x^+$ if keeping the same $\Delta x$. However this effect is very small in our case, therefore we keep the same $\Delta x$, $\Delta y$ and $\Delta z$ for the different temperature condition at the same Mach number. The grid details are shown in Table 2.

<table>
<thead>
<tr>
<th>Table 2: Details of Grid</th>
</tr>
</thead>
<tbody>
<tr>
<td>A3</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>$\Delta x^+$</td>
</tr>
<tr>
<td>$\Delta y^+$</td>
</tr>
<tr>
<td>$\Delta z^+$</td>
</tr>
<tr>
<td>$\Delta x/\delta$</td>
</tr>
<tr>
<td>$\Delta y/\delta$</td>
</tr>
<tr>
<td>$\Delta z/\delta$</td>
</tr>
</tbody>
</table>

where A and I stand for the adiabatic and isothermal cases, respectively and the number followed indicates the Mach number. The $\Delta x^+, \Delta y^+$ and $\Delta z^+$ are measured at the wall and the $\Delta x$, $\Delta y$ and $\Delta z$ are measured at $y/\delta = 1.0$. The grid is uniform in $x$ and $z$ directions and stretched in $y$ direction with about 23 layers of tetrahedra in the boundary layer for each case.

The initial condition is a turbulent mean profile with random fluctuations. The simulation is run first for 90 inertial timescales $\delta/U_\infty$ in order to eliminate starting transients (Lund et al 1998).

For a function $f$, its average in time form $<f>$ is defined by

$$
<f> = \frac{1}{t_f - t_i} \int_{t_i}^{t_f} f \, dt
$$

and its time fluctuating part is

$$
f'' = f - <f>
$$

In order to provide converged data, the primitive variables are averaged in spanwise direction and the statistical evaluations are performed on a period longer than $t_f - t_i = 40\delta/U_\infty$. The notation for the combined temporal and spanwise average is

$$
\ll f \gg = \frac{1}{L_z} \frac{1}{t_f - t_i} \int_{0}^{L_z} \int_{t_i}^{t_f} f \, dt \, dz
$$

A simplifying notation is used for the velocity, temperature and pressure

$$
U = \ll u \gg
$$

The mean streamwise velocity profiles using the Van Driest transformation are plotted in Fig. 3 and Fig. 4 (where $u_r$ is obtained from the simulation). Good agreement is shown with the viscous sublayer linear approximation $U_{VD}/u_r = y^+$ and Law of the Wall formulated in (1).
The mean velocity profiles shown in Fig. 5 and Fig. 6 exhibit virtually identical distributions for adiabatic and isothermal cases and show good agreement with experiment (Zheltovodov et al. 1986, Zheltovodov et al. 1990). The mean temperature profiles in Fig. 7 and Fig. 8 display a higher temperature distribution for the isothermal case with the wall temperature higher than the adiabatic and experiment data (Zheltovodov et al. 1990) which are also obtained at the adiabatic boundary condition. The difference is expected since the wall temperature for the isothermal case is fixed at 10% higher than the adiabatic case.

The discrepancies between Mach 4 cases and experiments in Fig. 6 and Fig. 8 are due to the effects of Mach number and Reynolds number. The Reynolds number in the simulation is one magnitude lower than experiments due to the significant computation cost in LES. The outer portion of the velocity profiles in Fig. 6 is in good agreement with experiment since this portion is not sensitive to the Reynolds number. The discrepancy in the inner portion is due to the effect of the Reynolds
number. The effect of Mach number is observed in Fig. 8, which can be explained using Crocco's relationship between the mean temperature and mean velocity profiles

\[
\frac{T}{T_\infty} = \frac{T_w}{T_\infty} + \frac{T_{aw} - T_w}{T_\infty} \frac{U}{U_\infty} - r \frac{\gamma - 1}{2} M_\infty^2 \left( \frac{U}{U_\infty} \right)^2
\]

where \(r\) is the recovery factor defined as

\[
r = \frac{T_r - T_\infty}{T_0 - T_\infty}
\]

where \(T_r\) is the adiabatic or recovery temperature and \(T_0\) is the freestream stagnation temperature. For the adiabatic case, Eq. (3) becomes

\[
\frac{T}{T_\infty} = \frac{T_w}{T_\infty} - r \frac{\gamma - 1}{2} M_\infty^2 \left( \frac{U}{U_\infty} \right)^2 \tag{5}
\]

Eqs. (3) and (5) show the trend that under the same mean velocity distribution, the mean temperature decreases with increasing Mach number, leading to the discrepancy between the calculation and experiment in the outer portion of the mean temperature profiles in Fig. 8. The discrepancy in the inner portion is mainly due to the effect of the Reynolds number.

The mean streamwise resolved turbulent kinematic normal stress \( \ll u''u'' \gg \), normalized using the local mean density \( \ll \rho \gg \) and wall shear stress \( \tau_w \), is shown in Fig. 9 and Fig. 10. As discussed in Zheltovodov and Yakovlev (1986) and Smits and Dussauge (1996), the scaling \( \ll \rho \gg \ll u''u'' \gg / \tau_w \) provides an approximate self-similar correlation of experimental data for supersonic flat plate zero pressure gradient adiabatic boundary layers, although the measurements close to the wall are subject to considerable uncertainty. In those two figures data are displayed from Konrad and Smits (1998), Johnson and Rose (1975), Muck et al (1984, 1985), Konrad (1993), as well as upper and lower bounds of an extensive set of experimental data for the Mach number range \( M = 1.72 \) to 9.4 in accordance with generalizations of Zheltovodov and Yakovlev (1986). The characteristics of the different experiments are displayed in Table 3. The computed results show good agreement with experiment for the main part of the boundary layer (\( y/\delta > 0.2 \)), despite a significantly higher
Table 3: Flat Plate Boundary Layer Experimental Data

<table>
<thead>
<tr>
<th>Name</th>
<th>Mach No.</th>
<th>Re_δ</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES</td>
<td>3.0 &amp; 4.0</td>
<td>20 × 10^3</td>
</tr>
<tr>
<td>DNS Adams (1997)</td>
<td>3.0</td>
<td>25 × 10^3</td>
</tr>
<tr>
<td>Johnson &amp; Rose (1975)</td>
<td>2.9</td>
<td>1000 × 10^3</td>
</tr>
<tr>
<td>Konrad (1993)</td>
<td>2.9</td>
<td>1590 × 10^3</td>
</tr>
<tr>
<td>Konrad &amp; Smits (1998)</td>
<td>2.87</td>
<td>1900 × 10^3</td>
</tr>
<tr>
<td>Muck et al (1984, 1985)</td>
<td>2.87</td>
<td>1638 × 10^3</td>
</tr>
<tr>
<td>Zheltovodov et al (1986)</td>
<td>1.7-9.4</td>
<td>up to 2000 × 10^3</td>
</tr>
</tbody>
</table>

experimental Reynolds number. The decreasing slope corresponds precisely to Johnson and Rose (1975) data. For \( y/δ < 0.2 \) the presence of the typical high level peak in the near wall region is supported by experimental data of Konrad (1993) and the Direct Numerical Simulation data from Adams (1997), which is nearly at the same Reynolds number as the LES. However, no conclusion can be drawn about the precise \( y \) position and the width of this peak without further experimental data or DNS.

Figure 9: Streamwise Reynolds stress at M=3  Figure 10: Streamwise Reynolds stress at M=4

In Fig. 11 and Fig. 12 Reynolds shear stress distributions are shown for the same experiments and the DNS. Again, the data fit well in the outer part of the boundary layer. The maximum value and the decreasing slope are again well predicted.

The capability of our LES method to accurately predict the heat transfer in the flat plate boundary layer is evaluated. The Reynolds analogy relates the skin friction coefficient \( C_f \) and heat transfer coefficient \( C_h \) by the Prandtl number as follows

\[
\frac{2C_h}{C_f} = \frac{1}{Pr_{tm}}
\]  

(6)

where \( C_h \) and \( C_f \) are written as

\[
C_h = \frac{q_w}{\rho_\infty U_\infty c_p(T_w - T_{aw})}
\]  

(7)
Figure 11: Reynolds shear stress at M=3

Figure 12: Reynolds shear stress at M=4

\[ C_f = \frac{\tau_w}{\frac{1}{2} \rho \infty U_{\infty}^2} \]  \hspace{1cm} (8)

where \( c_p \) is the specific heat at constant pressure. The wall heat flux \( (q_w) \) and skin friction \( (\tau_w) \) are obtained from the isothermal case and the adiabatic wall temperature \( (T_{aw}) \) is calculated from the adiabatic case. The wall heat flux is

\[ q_w = -\lambda \frac{\partial T}{\partial y} \bigg|_w \]  \hspace{1cm} (9)

and the wall shear stress is

\[ \tau_w = \mu_w \frac{\partial u}{\partial y} \bigg|_w \]  \hspace{1cm} (10)

Table 4: LES predictions

<table>
<thead>
<tr>
<th>Name</th>
<th>( T_w/T_{\infty} )</th>
<th>( C_f )</th>
<th>( C_h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A2.88</td>
<td>2.51</td>
<td>( 2.44 \times 10^{-3} )</td>
<td>0</td>
</tr>
<tr>
<td>I2.88</td>
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<td>( 1.27 \times 10^{-3} )</td>
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<td>A4</td>
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</tr>
<tr>
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<td>4.23</td>
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<td>( 1.24 \times 10^{-3} )</td>
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</table>
Table 5: Comparison of LES and Experiment

<table>
<thead>
<tr>
<th>Cases</th>
<th>Name</th>
<th>LES</th>
<th>Experiment</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach=2.88</td>
<td>$T_{aw}/T_{\infty}$</td>
<td>2.51</td>
<td>2.549</td>
<td>1.5%</td>
</tr>
<tr>
<td></td>
<td>$C_f$</td>
<td>$2.32 \times 10^{-3}$</td>
<td>$2.56 \times 10^{-3}$</td>
<td>9.4%</td>
</tr>
<tr>
<td></td>
<td>$C_h$</td>
<td>$1.27 \times 10^{-3}$</td>
<td>$1.44 \times 10^{-3}$</td>
<td>11.8%</td>
</tr>
<tr>
<td></td>
<td>$2C_h/C_f$</td>
<td>1/0.91</td>
<td>1/0.89</td>
<td>2.2%</td>
</tr>
<tr>
<td></td>
<td>$Pr_{tm}$</td>
<td>0.91</td>
<td>0.89</td>
<td>2.2%</td>
</tr>
<tr>
<td>Mach=4.0</td>
<td>$T_{aw}/T_{\infty}$</td>
<td>3.95</td>
<td>3.848</td>
<td>2.6%</td>
</tr>
<tr>
<td></td>
<td>$C_f$</td>
<td>$2.0 \times 10^{-3}$</td>
<td>$2.17 \times 10^{-3}$</td>
<td>7.8%</td>
</tr>
<tr>
<td></td>
<td>$C_h$</td>
<td>$1.24 \times 10^{-3}$</td>
<td>$1.22 \times 10^{-3}$</td>
<td>1.6%</td>
</tr>
<tr>
<td></td>
<td>$2C_h/C_f$</td>
<td>1/0.81</td>
<td>1/0.89</td>
<td>9.9%</td>
</tr>
<tr>
<td></td>
<td>$Pr_{tm}$</td>
<td>0.81</td>
<td>0.89</td>
<td>9.0%</td>
</tr>
</tbody>
</table>

Note:

Experimental $T_{aw}$ from Eq. (3)
Experimental $C_f$ from Eqs. (1), (2) and (8)
Experimental $C_h$ from Eq. (6)

The wall temperature $T_w$ is fixed at $T_w = 1.1 T_{aw}$, where the empirical adiabatic wall temperature $T_{aw} = [1 + (7/2) Pr_{tm} M_{\infty}^2]T_{\infty}$. All the predicted results are listed in Table 4, where the wall temperature for the isothermal case is fixed. The comparison with experiment is shown in Table 5. The experimental adiabatic wall temperature is computed from $T_{aw} = [1 + (7/2) Pr_{tm} M_{\infty}^2]T_{\infty}$. The computed mean turbulent Prandtl number from (6) shows good agreement with experiment value of 0.89, indicating the consistency of LES results with the Reynolds analogy.

The turbulent Prandtl number changes across the boundary layer. Simpson et al (1970) have established the uncertainty envelope of the turbulent Prandtl number for incompressible zero pressure gradient turbulent boundaries. The experimental predictions by Meier and Rotta (1971) at Mach number up to 4.5 at the wall and Horstman and Owen (1972) at M=7.2 and cooled wall conditions fall into this uncertainty envelope. According to the eddy viscosity hypothesis, the turbulent stress and heat flux can be expressed as

$$\tau_{ik} = -\rho u'_i u'_k = \mu_t \frac{\partial \bar{u}_i}{\partial x_k} + \frac{2}{3} \frac{\partial \bar{u}_i}{\partial x_j} \delta_{ik}$$  \hspace{1cm} (11)

$$Q_k = -c_p \rho T' u'_k = \lambda \frac{\partial \bar{T}}{\partial x_k}$$  \hspace{1cm} (12)

where the bar denotes the filtered flow variables and the tilde denotes the Favre-averaged filtered flow variables. The local turbulent Prandtl number ($Pr_t$) for a two-dimensional boundary layer can be derived from the above two equations as

$$Pr_t = \frac{\frac{\partial \bar{T}}{\partial y} \rho u' v'}{\frac{\partial \bar{u}'}{\partial y} \rho T' v'}$$  \hspace{1cm} (13)

The calculated turbulent Prandtl number profile is shown compared with the experimental range in Fig. 13. The Prandtl number reaches the maximum at the wall and starts to decrease away from the wall. In the outer portion of boundary layer, the fluctuation of Prandtl number is relatively greater than the inner portion, which is consistent with the experimental trend.
2 Compression Corner

Supersonic flow past a compression corner is an important problem in aerodynamics. It represents, for example, the deflection of a control surface on a wing. The shock can cause a boundary layer separation upstream of the point of impingement of the primary shock, with a secondary shock forming near the separation (Andreopoulos and Muck 1987, Dolling and Or 1983, Horstman et al 1977, Settles et al 1979, Smits and Muck 1987, Zheltovodov et al 1983, Zheltovodov and Yakolev 1986, and Zheltovodov 1996). Reynolds-averaged Navier-Stokes simulations have failed to accurately predict the flow characteristics (Knight and Degrez 1998) such as fluctuating pressure and heat transfer.

2.1 Weighting Function and Limiters

The computation of a strong shock using the exact Riemann solver (Godunov's method) and the Least Squares method (Ollivier 1997) as a reconstruction scheme leads to the generation of oscillations in the vicinity of shock waves which cause numerical instability. It can be shown theoretically that a linear second-order upwind scheme always generates oscillations. The only way to overcome this limitation, while satisfying the concept of an entropy function, is to introduce non-linear components. The classical method to avoid such spurious oscillations is to implement limiters which control the gradient of the computed quantities to prevent the appearance of overshoots and undershoots. An excellent review of this technique is described in Hirsh 1997. A different approach is the stencils-searching ENO schemes which have been extended to unstructured grids (Abgrall 1994). At each time step, the stencil is chosen which provides the smoothest reconstruction. However, this approach is computationally expensive for LES since it implies a determination of the stencil at every time step. Recently, Ollivier-Gooch (Ollivier 1997) proposed a weighted stencil method wherein the stencil is fixed but the weights are recomputed at each time step as required\(^1\).

\(^1\)We found that the weighted stencil method of Ollivier-Gooch (Ollivier 1997) provided an improvement compared to the unweighted results, but was nonetheless very sensitive to the weighting parameters. For the 25° compression corner, we found that overshoots and undershoots in the vicinity of the shock could not be avoided without adversely
2.2 Limiters

We consider limiters which control the gradient of computed quantities reconstructed to a cell face (denoted by the index \( i + \frac{1}{2} \)). The limiters described in the literature (e.g., Van Leer’s limiter, Minmod, Roe’s Superbee limiter) are expressed as a function of the ratio \( r_{i+\frac{1}{2}} \) of consecutive variations

\[
r_{i+\frac{1}{2}} = \frac{u_{i+1} - u_i}{u_i - u_{i-1}}
\]

This expression is well defined in case of a structured grid, where \( i + 1 \) means the next cell in the \( i \) discretization and \( i - 1 \) means the previous one.

2.3 Homogeneous Limiter

Consider a linear reconstruction of a flow variable wherein the computed gradient yields an overshoot (or undershoot) in the reconstructed value at the cell interface (Fig. 14). The overshoot (or undershoot) can be avoided if the interface values were to remain between the adjacent cell averaged values. We can limit the slope computed by the LS method to satisfy this criterion. For a one dimensional case, the interface value computed from the left cell \( i \) is

\[
u_{i+\frac{1}{2}}^{left} = u_i + C_i (x_{i+\frac{1}{2}} - x_i)
\]

where \( C_i = \partial u/\partial x \). Consider the case \( u_i \leq u_{i+1} \). Referring to Fig. 14, the reconstructed value \( u_{i+\frac{1}{2}}^{left} \) is required to lie within the adjacent cell averaged values

\[
u_i \leq u_{i+\frac{1}{2}}^{left} \leq u_{i+1}
\]

or

\[
0 \leq C_i \leq \frac{u_{i+1} - u_i}{x_{i+\frac{1}{2}} - x_i}
\]

This is achieved by replacing the gradient \( C_i \) by \( \eta C_i \) where

\[
\eta = \left\{ \begin{array}{ll}
1 & \text{for } 0 \leq C_i \leq \frac{u_{i+1} - u_i}{x_{i+\frac{1}{2}} - x_i} \\
\frac{u_{i+1} - u_i}{C_i (x_{i+\frac{1}{2}} - x_i)} & \text{for } C_i > \frac{u_{i+1} - u_i}{x_{i+\frac{1}{2}} - x_i} \\
0 & \text{for } C_i < 0
\end{array} \right.
\]

An analogous result can be obtained for the case \( u_i > u_{i+\frac{1}{2}} \).

For a general 3D configuration, the limited quantities are

\[
u_{i,j}^{left} = u_i + \eta \vec{C} \cdot \vec{\Delta x}
\]

where \( u_{i,j}^{left} \) is the reconstructed value of variable \( u \) for cell \( i \) and the face adjacent to cell \( j \), and

\[
\vec{C} \cdot \vec{\Delta x} = \begin{pmatrix} Cx_i \\ Cy_i \\ Cz_i \end{pmatrix} \cdot \begin{pmatrix} x_{i,j} - x_i \\ y_{i,j} - y_i \\ z_{i,j} - z_i \end{pmatrix}
\]

affecting the undisturbed boundary layer.
\[ \eta = \begin{cases} 
1.0 & \text{for } 0 \leq \vec{C} \cdot \Delta x \leq u_j - u_i \\
\frac{u_j - u_i}{\vec{C} \cdot \Delta x} & \text{for } \vec{C} \cdot \Delta x > u_j - u_i \\
0 & \text{for } \vec{C} \cdot \Delta x < 0 
\end{cases} \] (21)

The above expression holds for \( u_i \leq u_j \). An analogous expression holds for \( u_i > u_j \). In practice the limiter is successively applied to the different cell neighbors \( j \) of the cell \( i \). As far as tetrahedras are concerned, only the neighbors sharing a face are used.

A 25° compression corner computation has been designed to evaluate the efficiency of the limiter. Fig. 15 displays the evolution of the static temperature across the shock computed using the second order LS without a limiter. Strong overshoots and undershoots appear. Fig. 16 displays the static temperature in the shock using this limiter. The spurious oscillations disappear, although the gradients within the cells appear to have been reduced probably more than necessary.

### 2.4 Inhomogeneous Limiter

The homogeneous limiter (21) does not treat the function gradients \( Cx_i, Cy_i, Cz_i \) independently, and therefore is overly limiting. Consider a case where \( Cx_i \) and \( Cy_i \) are “satisfactorily” computed but \( Cz_i \) is overestimated by the LS method and therefore \( u_{i,j}^{left} \) is also overestimated. During the limitation process \( \eta \) is set to a value less than 1 because \( \vec{C} \cdot \Delta x \) is too large. As a result, all three gradients are reduced, even though \( Cx, Cy \) were “satisfactory”.

A three parameter limiter is defined by

\[ u_{i,j}^{left} = u_i + \left( \frac{\eta_x Cx_i}{\eta_y Cy_i} \right) \cdot \left( \frac{x_{i,j} - x_i}{y_{i,j} - y_i} \right) \] (22)

wherein each gradient \( Cx_i, Cy_i, Cz_i \) has a limiter. We present the inhomogeneous limiter for \( u_i \leq u_j \). Analogous expressions hold for \( u_i > u_j \).
Case 1: \( \vec{C} \cdot \Delta \hat{x} > u_j - u_i \)

\[
\eta_x = 1.0 - k_1 \left| \frac{C_{x_i}(x_{i,j} - x_i)}{k_2} \right| \\
\eta_y = 1.0 - k_1 \left| \frac{C_{y_j}(y_{j,i} - y_j)}{k_2} \right| \\
\eta_z = 1.0 - k_1 \left| \frac{C_{z_i}(z_{i,j} - z_i)}{k_2} \right| 
\]

(23)

where

\[
k_1 = \frac{\hat{u}_{i,j} - u_j}{\hat{u}_{i,j} - u_i} 
\]

(24)

\[
k_2 = \max \left\{ \frac{C_{x_i}(x_{i,j} - x_i)}{\Delta x}, \frac{C_{y_j}(y_{j,i} - y_j)}{\Delta y}, \frac{C_{z_i}(z_{i,j} - z_i)}{\Delta z} \right\} 
\]

(25)

where \( \hat{u}_{i,j} \) is the reconstructed value assuming \( \eta_x = \eta_y = \eta_z = 1 \).

Case 2: \( 0 \leq \vec{C} \cdot \Delta \hat{x} \leq u_j - u_i \)

\[
\eta_x = 1 
\]

(26)

\[
\eta_y = 1 
\]

(27)

\[
\eta_z = 1 
\]

(28)

Case 3: \( \vec{C} \cdot \Delta \hat{x} < 0 \)

\[
\eta_x = 0 
\]

(29)

\[
\eta_y = 0 
\]

(30)

\[
\eta_z = 0 
\]

(31)

The process mainly limits the components \( \eta_x, \eta_y, \eta_z \) whose contribution in the \( \vec{C} \cdot \Delta \hat{x} \) expression is the largest. When the \( j \) neighbor position is aligned with \( x, y \) or \( z \) direction, then only \( C_x, C_y \) or \( C_z \) is respectively reduced.

Fig. 17 displays the results of this limiter for the static temperature profile within the shock. The effect on the gradient is less severe than in Fig. 16. The 25° compression corner computations described below use this limiter.

2.5 ENO scheme

The key idea of ENO schemes is to use the smoothest stencil among several candidates to approximate the fluxes at cell boundaries to a high order accuracy and at the same time to avoid spurious oscillations near shocks. We previously computed supersonic turbulent flow past compression corner of 8° at Mach 3 without use of limiters (Urbin 1999). However, the 25° compression corner at Mach 3 (see Fig. 18) requires a limiter, and thus determination of the most effective limiter is the objective of this part of our study. In the 25° compression corner, a strong shock is formed through a series of unsteady compression waves, and variations in the flow variables in the boundary layer are sometimes comparable to the shock. In order to determine a proper criterion to construct the ENO stencil, we begin with the analysis of the variable gradient (we use density since it has a similar change as the other variables), shown in Fig. 19 at \( x = 3\delta \), where \( x \) is measured from the corner and \( \delta \) is the inflow boundary layer thickness. The density is non-dimensionalized by the
freestream density $\rho_\infty$. The gradient using the isotropic stencil (Okongo 1998) with Least Squares reconstruction shows two peaks corresponding to the boundary layer and the shock wave. Outside these two regions, the change of the gradient is smooth. The selection of the ENO stencil should take advantage of this feature and make the ENO stencil focus on these two regions.

First, we establish a criterion to decide where to use the ENO stencil. The density ratio across the shock is approximately 2.19 according to the Rankine-Hugoniot equations. The maximum norm of the density gradient $\alpha$ is approximately equal to 6 with mesh spacing $\Delta r = \sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2} = 0.2$ in the vicinity of the shock, where $\Delta r$ is non-dimensionalized by $\delta$. We make a cut-off at $\alpha = 6$ and any cell whose density gradient is larger than $\alpha$ should use an ENO stencil. We define $\Sigma$ as a set of cells satisfying $|\nabla \rho| > \alpha$. In Fig. 19, the maximum density gradient based on the isotropic stencil is approximately 13.

Second, for all $\Sigma$, a direction should be found to construct the ENO stencil. Consider any tetrahedron in $\Sigma$ in which four possible density gradients are computed using only three face neighbors, denoted as $|\nabla \rho|_k$ ($k = 0, 1, 2, 3$). The subscript is the index of the face neighbor which has been excluded. The density gradients are computed by the Least Squares method. We assume that

$$ |\nabla \rho|_3 \geq |\nabla \rho|_2 \geq |\nabla \rho|_1 \geq |\nabla \rho|_0 $$

where $|\nabla \rho|_{\max} = |\nabla \rho|_3$, $|\nabla \rho|_{\min} = |\nabla \rho|_0$.

We construct the ENO stencil as follows. First, the three face neighbors which give the minimum density gradient are added. Second, we find all the node neighbors of any cell of $\Sigma$ and exclude all the cells which share at least one node with the remaining face neighbor. Any five of the remaining cells which are the node neighbors of that cell and these three face neighbors are used to construct the ENO stencil.

A modified Riemann shock tube case with the initial pressure ratio of ten and an initial distribution of isotropic turbulence is used to verify the ENO scheme and to compare with the inhomogeneous limiter. The pressure ratio across the shock is chosen close to that in the 25° compression corner. The cut-off number $\alpha$ is set to 6. Fig. 20 shows the comparison between the inhomogeneous limiter and the ENO scheme for the Riemann shock tube case. It can be seen that the ENO stencil is
Figure 19: $|\nabla \rho|$ vs $y/\delta$

Figure 20: ENO cells for a Riemann shock tube

Figure 21: ENO cells for 25° compression corner

Figure 22: Flowfield behaviour across shock
used only in the shock region, while the inhomogeneous limiter is also used in the expansion fan region where there are no overshoots and even in the undisturbed flow in presence of turbulence. In Fig. 21, the ENO scheme is applied to the 25° compression corner with $\alpha = 6$. The cells using the ENO stencil appear principally in the shock region and the boundary layer downstream of the corner where the density gradient has a larger variation than the upstream. Fig. 22 shows the instantaneous profiles of velocity and pressure along the direction perpendicular to the shock wave at $z = 1.0\delta$ (where $y_e$ is measured along the direction perpendicular to the shock wave and $U_\infty$ is the streamwise velocity in the freestream.). The $x$ coordinate of the interception point of the $y_e$ with the solid wall is $5\delta$, where $x$ is measured from the corner. The shock wave is efficiently limited within the width of two or three cells.

2.6 Results

David (1993) performed the first LES of a compression corner which successfully reproduced the Taylor-Görtler vortices downstream of the shock. Nevertheless, the use of a pseudo-compressible subgrid-model did not permit accurate quantitative results. The second and most recent LES was Hunt and Nixon (1995) who investigated the role played by turbulence, and showed a direct correlation between the shock motion and the incoming velocity fluctuations. They also demonstrated that the size of the separation bubble has, to some extent, a weak effect on the shock motion. Despite the lack of detail in the inner layer (a log-law wall function was used on a rough grid resolution), it displayed the qualitative features of the shock oscillation observed experimentally (Dolling and Or 1983).

A computation of an adiabatic turbulent boundary layer flow past a 25° compression corner at Mach 3.0 and $Re_\delta = 2 \times 10^4$ was performed.

Allowing $x$, $y$, and $z$ to denote the streamwise, transverse and spanwise directions, respectively, the computational domain is $L_x = 16.0\delta$, $L_y = 3.4\delta$, and $L_z = 1.925\delta$. The grid consists of $213 \times 35 \times 57$ nodes in the $x$, $y$ and $z$ directions, respectively. The reference quantities for non-dimensionalization are length $\delta$ (the incoming boundary layer thickness), velocity $U_\infty$, density $\rho_\infty$, static temperature $T_\infty$ and molecular viscosity $\mu_\infty$ (where the subscript $\infty$ denotes the freestream conditions upstream of the compression corner). The tetrahedral grid is employed and stretched in the $y$ direction with a spacing of $0.008\delta$ at the wall and the stretching factor of 1.154. The grid is concentrated around the compression corner. The details of the grid are shown in Table 6, wherein $\Delta y^+ = \Delta y/\eta$ with

<table>
<thead>
<tr>
<th>Table 6: Details of Grids</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
</tr>
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<td>-------------------</td>
</tr>
<tr>
<td>Theoretical value</td>
</tr>
<tr>
<td>LES</td>
</tr>
</tbody>
</table>

the inner length scale $\eta = \nu_w/u_r$ ($\nu_w$ is the kinematic viscosity at the wall, $u_r = \sqrt{\tau_w/\rho_w}$ is the friction velocity, $\tau_w$ is the wall shear stress and $\rho_w$ is the density at the wall). The theoretical values of $u_r$ and $\nu_w$ are obtained from the combined Law of the Wall and Wake evaluated at $y = \delta$ and the power law of the relationship between temperature and kinematic viscosity, respectively.

The inflow condition is obtained from a separate flat plate boundary layer computation. The non-
slip boundary condition is used to the adiabatic wall. All the flow variables shown in the figures are averaged in time and the spanwise direction. The time averaging period is set to three times the flow-through time, where one flow-through time is defined as the time for the freestream flow to traverse the computational domain. The details are presented in Urbin et al 1999.

The oncoming flow characteristics are illustrated by the mean flow variables in Fig. 23 and Fig. 24 and the Reynolds shear stress in Fig. 25. The comparisons with experiments (Zheltovodov et al 1990) and DNS show good agreement.

Fig. 26 shows the pressure contour distribution at $x - y$ plane of $z = 1.0$. A strong separation and attachment shock wave is formed at the compression corner leading to the higher pressure level.
after the shock. The strong adverse pressure gradient causes the skin friction coefficient to decrease dramatically and the flow separates. Downstream of the corner, the overall increase in pressure and the decrease in Mach number cause the skin friction coefficient to recover.

![Figure 27: Skin friction coefficient](image1)

![Figure 28: Surface wall pressure](image2)

![Figure 29: Separation length for LES and DNS](image3)

The computational results are shown in Fig. 27–Fig. 29 along with experimental data. The skin friction coefficient in Fig. 27 is compared with the experiment at higher Reynolds number of $Re_\delta = 63560$. According to the Law of the Wall and Wake, the friction velocity is decreased with the increase in Reynolds number, leading to the higher skin friction coefficient in the computation. The time and spanwise averaged surface pressure profile along the streamwise direction is compared with experiment at higher Reynolds number in Fig. 28 and the pressure plateau is not observed. The difference between the predicted and experimental surface pressure profile may be attributable to the difference in Reynolds number.

The effect of Reynolds number on the separation length is plotted in Fig. 29. In this figure, the separation length is measured by connecting the separation and attachment points at which the
time and spanwise averaged skin friction coefficients go to zero and then scaled by the characteristic length \( L_c \) proposed by Zheltovodov and Schuelein 1987, 1993.

\[
L_c = \delta (p_2/p_{pl})^{3.1}/M_{\infty}^3
\]

(32)

where \( \delta \) is the incoming boundary layer thickness, \( p_2 \) is the pressure after the shock in inviscid flow, \( p_{pl} \) is the plateau pressure obtained by the empirical formula \( p_{pl} = p_{\infty}(0.5M_{\infty} + 1) \) (Zukoski 1967) and \( M_{\infty} \) is the Mach number in the uniform flow. Some LES and DNS results by other researchers are also plotted in Fig. 29 for comparison. Our LES successfully predicts the consistent trend with the experiment.

3 Expansion-Compression Corner

Supersonic expansion-compression corner (Fig. 30) is reminiscent of aerodynamic configurations wherein a supersonic boundary layer is subjected to an initial expansion followed by a subsequent compression. Interest in this configuration is due in part to the stabilizing influence of the expansion (Dussauge 1987, Zheltovodov et al 1987, Zheltovodov and Schuelein1987, Smith 1997, Stephen 1998, Zheltovodov 1990). The first systematic combined experimental and numerical study of an expansion-compression corner by Zheltovodov 1992 and Zheltovodov 1993 showed that several different turbulence models (including \( k-\epsilon, q-\omega \) and several modifications thereto) did not accurately predict the separation and attachment positions, and distributions of surface skin friction and heat transfer. We therefore seek to ascertain the capability of LES to predict this flowfield.

An incoming Mach 3 adiabatic equilibrium turbulent boundary layer of height \( \delta \) expands over a 25° corner followed by a 25° compression. The distance along the expansion surface is 7.1\( \delta \) \((i.e.,\) the vertical distance between the two horizontal surfaces is 3\( \delta \), and the horizontal distance between the expansion and compression corners is 6.43\( \delta \)).

The Cartesian coordinates \( x, y \) and \( z \) are aligned in the incoming streamwise, transverse and spanwise directions with the origin at the inflow boundary. The computational domain is \( L_x = 24.0\delta \), \( L_y = 3.4\delta \), and \( L_z = 1.925\delta \). The expansion corner is located at 4\( \delta \) from the inflow boundary. The grid consists of 253 \( \times \) 35 \( \times \) 57 nodes in the \( x, y \) and \( z \) directions, respectively, forming 479,808 hexahedra which are subdivided into five tetrahedra each. Thus, the total number of tetrahedra is 2,399,040. The grid is stretched in the \( y \) direction with spacing 0.008\( \delta \) at the wall and a geometric stretching factor of 1.154. The grid is concentrated in the streamwise direction in the neighborhood of the expansion and compression corners. The details are shown in Table 7 where \( \Delta y_+ = \Delta y/x_+ \nu_w \) where \( \nu_w \) is the computed kinematic viscosity at the wall, \( u_+ = \sqrt{\tau_w/p_w} \) is the friction velocity, \( \tau_w \) is the computed wall shear stress and \( \rho_w \) is the computed density at the wall. The grid is consistent with the resolution requirements for the LES code established by Urbin 2001.

<table>
<thead>
<tr>
<th>Name</th>
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<th>( \Delta z^+ )</th>
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<th>( \Delta y/\delta )</th>
<th>( \Delta z/\delta )</th>
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<td>Computed</td>
<td>20.9</td>
<td>1.67</td>
<td>7.1</td>
<td>0.1</td>
<td>0.14</td>
<td>0.034</td>
<td>2,399,040</td>
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<tr>
<td>at ( y = \delta )</td>
<td></td>
<td></td>
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The inflow boundary condition is obtained from a separate flat plate boundary layer computation. Experimental data has been obtained by Zheltovodov et al 1987, Zheltovodov and Schuelein 1987, Zheltovodov 1990a and presented in part in tabular form in Zheltovodov 1990 for the expansion-
compression corner at Mach 3 and several Reynolds numbers $Re_\delta$ based on the incoming boundary layer thickness $\delta$. The experimental conditions are listed in Table 8, where FPBL and ECC imply flat plate boundary layer and expansion-compression corner, respectively. The LES was performed at a lower Reynolds number ($Re_\delta = 2 \times 10^4$) than the experiment ($Re_\delta = 4.4 \times 10^4$ to $1.94 \times 10^5$) for reasons of computational cost. Additional LES cases will be performed at higher Reynolds numbers.

<table>
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<th>Cases</th>
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<th>References</th>
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<tr>
<td>ECC</td>
<td>2.9</td>
<td>$4.07 \times 10^4$</td>
<td>Zheltovodov 1990</td>
</tr>
<tr>
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<td>2.9</td>
<td>$6.76 \times 10^4$</td>
<td>Zheltovodov 1990</td>
</tr>
<tr>
<td>ECC</td>
<td>2.9</td>
<td>$8.0 \times 10^4$</td>
<td>Zheltovodov 1990</td>
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<tr>
<td>ECC</td>
<td>2.9</td>
<td>$1.94 \times 10^5$</td>
<td>Zheltovodov 1987 and Zheltovodov 1990a</td>
</tr>
<tr>
<td>ECC</td>
<td>2.88</td>
<td>$2.0 \times 10^4$</td>
<td>Present computation</td>
</tr>
<tr>
<td>FPBL</td>
<td>2.88</td>
<td>$1.33 \times 10^5$</td>
<td>Zheltovodov 1990a</td>
</tr>
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</table>

The structure of the flowfield is shown in Figs. 31 and Fig. 32 which display the mean static pressure and streamlines at $z = \delta$. The flow expands around the first corner, and recompresses at the second corner through a shock which separates the boundary layer as evident in Fig. 32. The flowfield structure is in good agreement with the results of Zheltovodov 1987, Zheltovodov 1988, Zheltovodov 1990 and Zheltovodov 1990a which are shown qualitatively in Fig. 30.

![Figure 31: Mean static pressure (s is separation, Figure 32: Mean streamlines (s is separation, A is attachment)](image)

![Figure 32: Mean streamlines (s is separation, A is attachment)](image)

The mean velocity profiles in the $x$-direction are shown in Fig. 33 at $x = 2\delta$ and $x = 6\delta$, where $x$ is measured from the inflow along the direction of the inflow freestream velocity (Fig. 31). The abscissa is the component of velocity locally parallel to the wall, and the ordinate is the distance measured normal to the wall. The first profile is upstream of the expansion corner which is located at $x = 4\delta$, and the second is downstream of the expansion fan and upstream of the separation point. The computed mean velocity profile at the first location is slightly fuller than the experiment. This is consistent with the experimentally observed dependence of the exponent $n$ in the power-law $U/U_\infty = (y/\delta)^{1/n}$ on the Reynolds number. The second profile shows a significant acceleration of
the flow in the outer portion of the boundary layer due to the expansion.

\[
L_c = \delta_e (p_2 / p_{pl})^{3.1} / M_e^3
\]  
(33)

where $\delta_e$ is the incoming boundary layer thickness (upstream of the expansion corner), $p_2$ is the pressure after the shock in inviscid flow, $p_{pl}$ is the plateau pressure from the empirical formula $p_{pl} = p_e (\frac{1}{2} M_e^2 + 1)$ where $p_e$ and $M_e$ are the static pressure and freestream Mach number upstream of the compression corner and downstream of the expansion fan. In the computation, the location is taken to be $x = 6\delta$. The values of $M_e$ and $p_2$ have been computed using inviscid theory. Also, $Re_{\delta_e} = 1.8 \times 10^4$ for LES ($Re_{\delta_e} = \rho_e U_e \delta_e / \mu_e$, where $\rho_e, U_e$ and $\mu_e$ are computed using inviscid theory). The experimental data correlation of Zheltovodov 1988 and the computed result\(^2\) for the scaled separation length is shown in Fig. 34. The computed value is consistent with a linear extrapolation of the experimental data.

The surface pressure profile in Fig. 36 displays a pressure plateau on the compression face generated by the separation bubble. The experiments exhibit a trend of increase in the size of the pressure plateau region with decreasing Reynolds number. The experimental data at the lowest Reynolds number ($Re_\delta = 4.1 \times 10^4$) shows close agreement with the computed results for $Re_\delta = 2 \times 10^4$ for the location, extent and magnitude of the pressure plateau. Moreover, the shape of the experimental pressure plateau shows little variation for $Re_\delta \leq 6.8 \times 10^4$, thus suggesting that the computed pressure plateau region (for $Re_\delta = 2 \times 10^4$) is accurate. The computed recovery of the surface pressure is more rapid than in the experiment, however.

\(^2\)The uncertainty in the computed value of $L_{sep}/L_c$ is associated with the uncertainty in determining $\delta_e$. We have used the streamwise Reynolds stress ($\ll \rho \gg \ll u' u' \gg$) to determine $\delta_e$ (Fig. 35), where $u'$ is the fluctuating velocity parallel to the wall.
The computed and experimental mean skin friction coefficient $c_f = \frac{\tau_w}{\frac{1}{2} \rho_\infty U_\infty^2}$ are shown in Fig. 37. The computed separation and attachment points are evident. The skin friction rises rapidly downstream of attachment. The computed results at $Re_\delta = 2 \times 10^4$ are in close agreement with the experimental data at $Re_\delta = 8.0 \times 10^4$ and $1.94 \times 10^5$ in the region downstream of reattachment.

Figure 35: Reynolds streamwise stress

Figure 36: Surface pressure

Figure 37: Skin friction coefficient
Turbulent round and plane jets are simple inhomogeneous flows that can be served to verify models for complex flows and have been experimentally and numerically studied extensively (Pancharapalan 1993, Rodi 1980). Recently, noncircular jets have been gained much interest in passive control due to their enhanced jet mixing properties (Grinstein 1992, Grinstein 1995a, Grinstein 1995b, Grinstein 2001, Gutmark 1999). A square jet at a Reynolds number of 3200 and a Mach number of 0.3 is simulated. Temporal evolutions are visualized to characterize the dynamics of deforming vortex rings, ribs and their interactions. Statistical quantities are quantified and compared with the DNS results of Grinstein et al. 1995.

The grid consists of $65 \times 65 \times 65$ hexahedral cells in an unstructured grid covering a computational domain of $5D$ in the streamwise direction and $\pm 3D$ along the transverse directions. Each hexahedral cell is divided into five tetrahedral cells, yielding a total of 1.3M tetrahedra. A uniform grid is used along the streamwise direction with the hexahedral grid spacing of $\Delta x/D = 0.078$, which is larger than 0.04 used by Grinstein et al. in their DNS (Grinstein 1995). The grids are stretched along the other two directions and the minimum grid spacings are $\Delta y/D = \Delta z/D = 0.0375$. The imposed boundary conditions include inflow, outflow and wall boundaries. At the inflow, the streamwise velocities are prescribed as

$$u = U[1 + A \sin(2\pi ft)]$$

and

$$U = 0.5 \ U_\infty \ [1 - \tanh[b_2(2|y|/D - D/(2|y|))] \times 0.5 \ U_\infty \ [1 - \tanh[b_2(2|z|/D - D/(2|z|))]],$$

where $A = 0.02$ is the perturbation amplitude, $f$ is the forcing frequency ($f = 0.5$), $b_2 = 0.25 R_{\frac{1}{2}}/\theta$, where $R_{\frac{1}{2}}/\theta = 40$, $R = D/2$ and $\theta$ is the momentum thickness. Zero-gradient condition is imposed at the outlet and symmetry boundary conditions are used at the side walls.

The iso-surfaces of the total vorticity $\omega = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$ corresponding to $\omega = 0.25 \omega_{peak}$ are shown in Fig. 38. Azimuthal nonuniformities make the evolution of the jet shear layer more complicated relative to circular jets. Close to the jet exit, a smooth square vortex sheet can be observed, and subsequently rolled-up vortex-ring structures form due to shear-layer Kelvin-Helmholtz instability. However, the vortex rings further downstream deform to non-planar shape due to self-induction mechanism caused by azimuthal nonuniformities. The deformed vortex rings are connected with the four corners of the initial square sheet by ribs. The hairpin braid vortices aligned with the corners progress faster in the diagonal direction than the others, “which results in redistribution of energy between azimuthal and streamwise vortices” (Grinstein 2001). Further downstream, the jet development is characterized by the strong interaction between vortex rings and braid vortices, which leads to a final breakdown of the large-scales coherent structures and transition to the turbulent flow. The self-induced deformation of the rings and rib pair were explained to be the leading mechanism for larger entrainment properties in non-circular jets relative to circular jets (Grinstein 1992). “The interactions between the streamwise vortices and the vortex rings is reminiscent of the interaction between ribs and spanwise rollers in the mixing layer” (Grinstein 1992). Mixing of jets with surroundings can be enhanced through controlling the formation, development and interaction of large-scale coherent structures passively.

Fig. 39 shows the instantaneous crosswise vorticity $\omega_x = \partial v/\partial x - \partial u/\partial y$ contours at the central $x - y$ plane. Rolled-up structures can be observed near the base, and subsequently symmetrical
counterrotating toroidal structures form in the shear layer which are then followed by their stretching and deformation. The organized structures can be broken down into smaller eddies further downstream. Evidently, the MILES model can capture the transition process. Large-scale vortex rings dominate in the near-field and the small vortices dominate downstream after the breakdown. The spatial spreading can be clearly observed downstream as the jet spreads by entraining mass from the surrounding nonvortical fluid.

Fig. 40 (a-d) shows the contours of instantaneous streamwise vorticity, $\omega_x = \partial v/\partial z - \partial w/\partial y$, across the $y - z$ planes of $x/D = 1, 2, 3$ and 4. Quite different behaviour can be observed at different axial positions. Vortex shears with some rounded-corners are stretched and thickened but still keep the initial square shape at the position of $x/D = 1$. The jet cross section switches axis $45^\circ$ relative to that of the jet nozzle at the axial location of $x/D = 2, 3$ due to self-induced velocity around the corners by the presence of streamwise vorticity. The flow structure develops into an irregular shape further downstream at $x/D = 4$.

The statistical quantities are obtained by averaging over five forcing cycles after a statistically stationary state has been reached after an elapsed dimensionless physical time of ten. The centerline distributions of the mean axial velocity by LES compared with the DNS results of Grinstein et al 1995 are plotted in Fig. 41. The mean velocity initially decays within the first 1.5 diameters and subsequently shows a slight increase due to the periodic roll-up by the sinusoidal forcing. The decay after 3.2 diameters is the result of turbulent mixing. In general, the agreement between present MILES and previous DNS results are good.

The corresponding centerline r.m.s. velocities $u'/U_c$ are shown in Fig. 42. Note that close to the inflow plane the r.m.s. of velocity fluctuations is about 2 percent and corresponds to the imposed disturbance level. In the potential core region, the r.m.s. velocity decreases slightly with increasing axial distance which shows a tendency to remain laminar with low turbulence intensities. Beyond the end of the potential core, the fluctuations of velocity increase very rapidly, which indicates the appearance of the secondary-instability mechanism which leads to the final breakdown of the large vortex structures. Due to insufficient length scale in the streamwise direction, the self-similar behaviour has not been achieved. However, it can be seen that the agreement between MILES and DNS is very good for the transient square jet.
Figure 38: Instantaneous isosurfaces of total vorticity $\omega = 0.25\omega_{peak}$.

Figure 39: Instantaneous streamwise vorticity contours at the $x-y$ centre-plane.
Figure 40: Instantaneous streamwise vorticity contours across the $y-z$ planes at $x/D = (a)$ 1, (b) 2, (c) 3 and (d) 4.

Figure 41: Centerline profiles of the mean velocity.

Figure 42: Centerline profiles of the r.m.s. axial velocity.
Personnel

The personnel of the research project are listed in Table 9.

<table>
<thead>
<tr>
<th>Name</th>
<th>Title</th>
<th>Period of Participation</th>
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<tr>
<td>Prof. Doyle Knight</td>
<td>Principal Investigator</td>
<td>Dec 98 - Mar 02</td>
<td>this grant and Rutgers</td>
</tr>
<tr>
<td>Dr. Frederic Thivet</td>
<td>Visiting Scientist</td>
<td>Dec 98 - Aug 00</td>
<td>ONERA</td>
</tr>
<tr>
<td>Dr. Gerald Urbin</td>
<td>Postdoctoral Associate</td>
<td>Dec 99 – Nov 99</td>
<td>this grant</td>
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<tr>
<td>Dr. Hong Yan</td>
<td>Research Associate</td>
<td>Sept 99 - Mar 02</td>
<td>this grant</td>
</tr>
<tr>
<td>Dr. Xu Zhou</td>
<td>Postdoctoral Associate</td>
<td>Nov 00 - Aug 01</td>
<td>this grant</td>
</tr>
</tbody>
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Journal Publications


Conference Publications


Knight, D., and Yan, H., “Large Eddy Simulation of Compressible Turbulent Flows”, West East
High Speed Flowfield Conference, Marseilles, France, April 2002.

Yan, H., Knight, D. and Zheltovodov, A., ”Large Eddy Simulation of Supersonic Flat Plate Boundary Layer Part II”, AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, July 7–10, 2002

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Johnson, D. and Rose, W. (1975) "Laser Velocimeter and Hot Wire Anemometer Comparison in a


