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Large Eddy Simulation of
Three-Dimensional High Speed Aerodynamic Flows

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Doyle Knight

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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: decay of isotropic turbulence, channel flow, supersonic flat plate boundary layer and supersonic compression corner. The first and second cases are effectively incompressible, while the third and fourth cases are supersonic (Mach 3). The computed results show close agreement with experiment and Direct Numerical Simulation, and validate the unstructured grid LES methodology.
# Table of Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction</td>
<td>4</td>
</tr>
<tr>
<td>Governing Equations</td>
<td>5</td>
</tr>
<tr>
<td>Numerical Algorithm</td>
<td>6</td>
</tr>
<tr>
<td>Parallelization</td>
<td>7</td>
</tr>
<tr>
<td>Results</td>
<td>7</td>
</tr>
<tr>
<td>Decay of Isotropic Turbulence</td>
<td>7</td>
</tr>
<tr>
<td>Channel Flow</td>
<td>9</td>
</tr>
<tr>
<td>Supersonic Flat Plate Turbulent Boundary Layer</td>
<td>12</td>
</tr>
<tr>
<td>Compression Corner</td>
<td>15</td>
</tr>
<tr>
<td>Bibliography</td>
<td>19</td>
</tr>
<tr>
<td>Personnel and Publications</td>
<td>23</td>
</tr>
</tbody>
</table>
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 (q_w and q'_w), mean surface skin friction (\tau_w), and locations of primary and secondary separation.

Table 1  RANS Capability for 3-D Shock Wave Boundary Layer Interaction

<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>
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<td></td>
<td></td>
</tr>
<tr>
<td>q_w</td>
<td></td>
<td>√</td>
<td></td>
</tr>
<tr>
<td>q'_w</td>
<td></td>
<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 Metais (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 Blaisdel (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 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 been 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: the decay of isotropic incompressible turbulence, channel flow, supersonic boundary layer and supersonic compression corner. 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 \( \tilde{f} \) is

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

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)

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial \rho}{\partial x_i} + \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} (\tilde{T} \tilde{u}_i)
\]

\[
\frac{\partial \rho \tilde{c}}{\partial t} + \frac{\partial \rho \tilde{c} \tilde{u}_i}{\partial x_i} = \frac{\partial \rho \tilde{Q}_k}{\partial x_k} + \frac{\partial}{\partial x_k} (\tilde{T} \tilde{u}_i)
\]

where

\[
T_{ik} = \tau_{ik} + \sigma_{ik}
\]

\[
\tau_{ik} = -\tilde{p}(u_i \tilde{u}_k - \tilde{u}_i \tilde{u}_k)
\]

\[
\sigma_{ik} = \mu(T) \left( -\frac{2}{3} \frac{\partial u_i}{\partial x_j} \delta_{ik} + \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right)
\]

\[
Q_k = Q_k + \tilde{q}_k
\]

\[
Q_k = -\rho c_p (\tilde{T} \tilde{u}_k - \tilde{u}_k)
\]

\[
\tilde{q}_k = k(T) \frac{\partial \tilde{T}}{\partial x_k}
\]

\[
\tilde{p} = \rho c_e \tilde{T} + \frac{1}{2} \tilde{p} \tilde{u}_i \tilde{u}_i + \tilde{k}
\]

\[
\frac{\partial \rho \tilde{k}}{\partial t} + \frac{\partial \rho \tilde{k}}{\partial x_i} = -\frac{1}{2} \tau_{ii}
\]
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

\[ \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial \tilde{z}_j} + \frac{\partial \tilde{u}_j}{\partial \tilde{z}_i} \right) \]

\[ \tau_{ij} = 2C_R \beta \Delta^2 \sqrt{\tilde{s}_{mn} \tilde{s}_{mn}} \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) \]

\[ Q_j = \tilde{\rho}c_p \frac{C_R}{Fr_t} \Delta^2 \sqrt{\tilde{s}_{mn} \tilde{s}_{mn}} \frac{\partial \tilde{T}}{\partial \tilde{z}_j} \]

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

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

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 and overbar. 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

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0 \]

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_k}{\partial x_k} = - \frac{\partial p}{\partial x_i} + \frac{\partial T_{ik}}{\partial x_k} \]

\[ \frac{\partial p_e}{\partial t} + \frac{\partial (p_e + p) u_k}{\partial x_k} = \frac{\partial}{\partial x_k} (Q_k + T_{ik} u_i) \]

\[ p = \frac{\rho T}{\gamma M_{\infty}^2} \]

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

\[ Q = \left\{ \begin{array}{c} \rho \\ \rho u \\ \rho v \\ \rho w \\ p_e \end{array} \right\} \]

and the flux vectors are

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

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 Prink (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 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).

**Results**

Four different configurations have been examined: decay of isotropic turbulence, channel flow, flat plate boundary layer and supersonic compression corner. The first and second cases are effectively incompressible, while the third and fourth cases are supersonic (Mach 3).

**Decay of Isotropic Turbulence**

The benchmark experiment by Comte-Bellot and Corrsin (CBC) (1971) of the decay of isotropic turbulence was selected to examine the following specific issues of the unstructured grid LES code: the MILES vs hybrid SGS models, the method for reconstruction of the flow variables to the cell faces, the demonstration of achieving consistent results using two different grids, the type of Riemann solver, regular vs random grids, the convergence parameter in Godunov’s method, and the number of Fourier intervals used in the initial spectrum. In the experiment, turbulence was generated using a biplane, square rod grid with mesh size \( M = 5.08 \text{ cm} \) and solidity of 0.34 in a uniform mean flow of velocity \( U_0 = 10 \text{ m/s} \). The Reynolds number based on the grid spacing is \( Re = 34000 \). The measurements were performed downstream of the grid at three locations, \( U_{0t}/M = 42, 98, \) and 171 where \( t \) is the dimensional “time” in the experiment. The computation was performed in a periodic box. Details are presented in Knight et al (1998).
Ten different computations, as summarized in Table 2, were performed to evaluate the issues described below. Cases 1 through 7 and 10 use the MILES model (i.e., no SGS model), while Cases 8 and 9 use the hybrid model (i.e., MILES plus the Smagorinsky SGS model). Case 1 employs a) second-order least-squares reconstruction with 8 cells in the stencil, b) a regular grid, c) Godunov’s method, d) a convergence parameter of $10^{-10}$ in Godunov’s method, and e) $N_k = 26$ in the initial energy spectrum. Cases 2 through 7 in succession modify one of these five choices. For example, Case 2 employs Frink’s method for reconstruction. Cases 8 and 9 use the hybrid (MILES plus Smagorinsky models) with different length scale $\Delta$. The Smagorinsky constant $C_R$ is chosen to be 0.012. Cases 1 to 9 employ Grid 1, and Case 10 employs Grid 2.

### Table 2 Decay of Isotropic Turbulence

<table>
<thead>
<tr>
<th>Case</th>
<th>Grid</th>
<th>SGS Model</th>
<th>$\Delta$</th>
<th>Reconstruction Method</th>
<th>Grid Type</th>
<th>$N_k$</th>
<th>Riemann Solver</th>
<th>Toler</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>MILES</td>
<td>n/a</td>
<td>LS 2nd</td>
<td>Reg</td>
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<td>Godunov</td>
<td>$10^{-10}$</td>
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<tr>
<td>2</td>
<td>1</td>
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<td>n/a</td>
<td>F 2nd</td>
<td>Reg</td>
<td>26</td>
<td>Godunov</td>
<td>$10^{-10}$</td>
</tr>
<tr>
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<td>Reg</td>
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<td>Roe</td>
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<td>Godunov</td>
<td>$10^{-10}$</td>
</tr>
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<td>n/a</td>
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<td>Godunov</td>
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</tr>
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<td>52</td>
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<tr>
<td>8</td>
<td>1</td>
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<td>F 2nd</td>
<td>Reg</td>
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<td>Godunov</td>
<td>$10^{-10}$</td>
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<td>F 2nd</td>
<td>Reg</td>
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<tr>
<td>10</td>
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<td>F 2nd</td>
<td>Reg</td>
<td>26</td>
<td>Godunov</td>
<td>$10^{-10}$</td>
</tr>
</tbody>
</table>

**Legend**

- **Grid 1**: No. of tetrahedra = 163,840
- **Grid 2**: No. of tetrahedra = 1,310,720
- **MILES**: Monotone Integrated Large Eddy Simulation (Boris et al. 1992)
- **LS 2nd**: Second order least-squares reconstruction method
- **F 2nd**: Second order Frink’s reconstruction method
- **First**: First order reconstruction method
- **Reg**: Regular grid of tetrahedra
- **Ran**: Grid obtained by random perturbing the nodes of the regular grid
- **$N_k$**: Number of Fourier intervals used for initial energy spectrum
- **Toler**: Tolerance employed in iteration solution for $p^*$

The decay of the resolved turbulence kinetic energy for Cases 1 to 9 is compared with the filtered experimental data of CBC in Fig. 2. The MILES method used either second order reconstruction method (Cases 1 to 3, and 5 to 7) accurately predicts the turbulence decay. This remarkable result implies that the inherent numerical dissipation in the numerical algorithm (due to the finite order accuracy of the reconstruction and quadrature) provides a reasonable model of turbulent energy dissipation. The computations employing the hybrid (MILES plus Smagorinsky models) exhibit only a small difference compared to the MILES simulations, since the dissipation of turbulence energy is almost entirely a consequence of the numerical algorithm (MILES).

![Fig. 2 Filtered turbulent kinetic energy](image-url)
The computation using the second order least-squares method (Case 1) shows a lower decay rate than those using Frink’s method (Cases 2, 3, and 5 to 7). The second order least-squares evidently has a lower inherent numerical dissipation than the second order Frink’s reconstruction. An SGS model may be needed to compensate the reduced inherent numerical dissipation in order to achieve the best agreement with experiment. The computation using the first order reconstruction (Case 4) shows poor agreement with experiment as anticipated.

The MILES approach yields consistent results when the grid is refined (Knight et al 1998). The results using either Roe’s method (Case 3) or Godunov’s method (Case 2) are essentially identical. This is expected since the velocity fluctuations are small compared to the speed of sound.

The choice of regular vs random grids has no significant effect on the accuracy of the computation as seen in Fig. 2, where the turbulence energy for Cases 2 and 5 are essentially identical. Moreover, the variation in the convergence parameter used in Godunov’s method (Cases 2 and 6), and the number of Fourier intervals in the initial condition (Cases 2 and 7) have negligible effect.

![Fig. 3 Energy spectrum at $U_0/M = 98$](image)

![Fig. 4 Energy spectrum at $U_0/M = 171$](image)

The effect of the functional reconstruction method on the turbulence energy spectrum is shown in Figs. 3 and 4 where the experimental data and computed results using the second order least-squares and Frink’s method are shown at $U_0/M = 98$ and 171, respectively, for Grid 1. The least-squares reconstruction is observed to be more accurate than Frink’s method. Since the CPU time for the two methods is approximately the same, the least-squares reconstruction is preferable. A “pile-up” of energy at lower wave numbers is noted. This was also observed by Haworth and Jansen (1996) who employed a similar grid resolution.

**Channel Flow**

The Reynolds number based on the channel height and bulk velocity is 5600. The Mach number is 0.5; however, the static temperature variation across the channel is small (less than 4%) so the flow is effectively incompressible. The mean flow is in the $x-$ direction, with $y$ and $z$ representing wall normal and spanwise directions, respectively.

Computations have been performed using the constant-coefficient Smagorinsky sub-grid scale model ($C_R = 0.012, Pr_t = 0.4$). The coefficient $C_R$ is multiplied by the van Driest damping factor $1 - e^{-y^2/26}$ to integrate to the walls. The length scale $\Delta$ for the SGS model is the nodal spacing in the $y$-direction. A body-force is applied in this direction and is adjusted at each timestep to keep the bulk velocity constant. Using the global $z$-momentum conservation for fully developed flow, $f_1 = -2u_z^2$. The bulk velocity is also the reference velocity and so is set equal to 1. The boundary conditions are periodic in the streamwise ($x$) and spanwise ($z$) directions with no-slip boundaries in the wall-normal ($y$) direction, with isothermal walls.

The grid size is $2\pi \times 1 \times 2\pi/3$, where the lengths have been non-dimensionalized by the channel height. The grid has $65 \times 65 \times 65$ nodes (274,625 nodes), 1,310,720 cells, and 2,646,016 faces. The grid is stretched in the $y$-direction, with minimum spacing (at the walls) of 0.00278 and a maximum spacing (in the channel center) of 0.0457. The initial condition is obtained from interpolating the fully-developed solution on a grid with
33 × 65 × 33 nodes with the same wall-normal (y) spacing but double the streamwise and spanwise spacing. The flow has been simulated for about twenty-two flow-through times, with statistics accumulated over the last twelve flow-through times. (One flow-through time is the domain length in the z-direction divided by the bulk velocity, i.e., 2π.) The results are compared with the experimental results of Eckelmann (1974) and Kreplin and Eckelmann (1974) and Direct Numerical Simulation of Kim et al (1987). In the presentation of results, statistics are accumulated at all grid points. Planar averages are obtained by averaging at all points on planes parallel to the walls, thus making the statistics functions of the wall-normal (y) direction only.

The computed friction velocity, normalized by the bulk velocity, is \( u_r = 0.0594 \) which is within 8% of the DNS and experimental values of 0.0643. The planar average of the time-averaged streamwise velocity \( U \) is shown in Figs. 5 and 6. The centerline velocity is 1.155 which is within 0.6% of the experimental value of 1.162. The LES is close to the DNS in the near-wall region, but overshoots slightly in the core of the channel, consistent with the lower shear stress of the LES. Notably, the LES has excellent agreement with the experimental data of Eckelmann (1979), whose log-law of \( u^+ = 2.65 \ln y^+ + 5.9 \) is based on data at \( Re_c \) of 5600 and 8200. The LES \( Re_c \) of about 6470 is between these values. The experimental data points shown in Fig. 6 are for \( Re_c = 5600 \).

![Fig. 5 Mean velocity in entire channel](image)

![Fig. 6 Mean velocity in wall units](image)

Figs. 7, 8 and 9 compare the root-mean-square velocity fluctuations from the LES with the DNS results of Kim et al and the experimental results from Kreplin and Eckelmann (1979). In the experiment, \( Re_c = 7700 \) and \( Re_r = 388 \), which are slightly higher that the DNS \( Re_c = 6600 \) and \( Re_r = 360 \) and the LES \( Re_c = 6470 \) and \( Re_r = 330 \). The velocity fluctuations from the LES, DNS and experiment show generally good agreement. The streamwise fluctuations (Fig. 7) of the LES compare favorably with the experiment, but are slightly higher than the DNS. The LES wall-normal fluctuations to be lower than those of the experiment and DNS (Fig. 8); however, the DNS is also significantly lower than the experiment. The spanwise fluctuations (Fig. 9) show comparable agreement with experiment for the LES and DNS. The computed Reynolds stress, shown in Fig. 10, compares very well with the DNS.

![Fig. 7 Rms streamwise velocity fluctuations](image)

![Fig. 8 Rms normal velocity fluctuations](image)
The higher-order velocity statistics based on the resolved velocities are shown in Figs. 11 to 16. The skewness for the streamwise velocity is defined by $S(u') = \frac{\overline{u'u'u'}}{\overline{u'u}^3/2}$ and likewise for $v'$ and $w'$, where the bar denotes the time-average and the prime denotes fluctuation relative to the time-average. Fig. 11 shows the streamwise skewness from the LES to be larger than the DNS, particularly in the center of the channel. The reasons for the disagreement with DNS are under evaluation. However, the agreement for the wall-normal and spanwise skewness, Figs. 12 and 13, is excellent. The flatness for the streamwise velocity is defined by $F(u') = \frac{\overline{u'u'u'u'}}{\overline{u'u}^3/2}$ and likewise for $v'$ and $w'$. The streamwise statistics of the LES deviate from the DNS (Fig. 14), while the normal and spanwise flatness profiles, shown in Figs. 15 and 16, agree very well with the DNS.
The channel flow LES simulation is effectively MILES, implying that the SGS dissipation is attributable to the numerical algorithm. This is evident in Fig. 17 which shows the Smagorinsky eddy viscosity normalized by the molecular viscosity. The peak value of the Smagorinsky is less than 10% of the molecular viscosity and occurs in the middle of the channel. Thus, the Smagorinsky eddy viscosity does not significantly contribute to the energy dissipation which is due almost entirely to the numerical algorithm. This is a particularly important result and the first observation of this type for an unstructured grid computation of turbulent channel flow.

It is recognized that the above comparison between the DNS and the LES is not precise because the DNS has not been filtered onto the LES grid. However, for this case most of the energy is in the resolved scales, as shown by Fig. 17.

**Supersonic Flat Plate Turbulent Boundary Layer**

An adiabatic flat plate turbulent boundary layer at Mach 3 and Reynolds number $Re_\delta = 2 \times 10^4$ (based on the incoming boundary layer thickness $\delta$) has been computed. The Reynolds number based on the momentum thickness $\delta_m$ and wall viscosity $\mu_w$ is $Re_\delta = 600$. 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. 18). 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 $L_z = 4.4\delta$. The spanwise width $L_z$ is approximately six 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 experimental 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 grid resolution is 1,600,000 tetrahedral cells. The grid at the wall uses 101 x 65 nodes. The nodal grid is stretched uniformly in the $y$ using a geometric factor of 1.088. The height $\Delta h$ of the first cell adjacent to the boundary is less than one wall unit ($\Delta u_r/\nu_r < 1$ where $\nu_r$ is the kinematic viscosity at the wall, $u_r = \sqrt{\tau_r/\rho_r}$ is the friction velocity, $\tau_r$ is the wall shear stress and $\rho_r$ is the density at the wall). 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).

Fig. 19 shows the instantaneous temperature contours within the boundary layer. Large turbulent streak-like structures eject high temperature fluid outward the inner layer.

For a function $f$, its average in time form $\langle f \rangle$ is defined by

$$\langle f \rangle = \frac{1}{t_f - t_i} \int_{t_i}^{t_f} f \, dt$$

and its time fluctuating part is

$$f'' = f - \langle f \rangle$$

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

$$\langle \langle f \rangle \rangle = \frac{1}{L_z} \frac{1}{t_f - t_i} \int_0^{L_z} \int_{t_i}^{t_f} f \, dt \, dz$$

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

$$U = \langle \langle u \rangle \rangle$$

The predicted friction velocity is $u_r/U_\infty = 0.053$ (the friction coefficient is $c_f = 2.10 \times 10^{-3}$) which is within 3% of the theoretical value of 0.0544 based on the friction law obtained from the combined Law of the Wall and Wake (using the classical coefficients $\kappa = 0.41; C = 5.0; H = 0.55$). The uncertainty in the experimental data of skin friction is typically $\pm 5\%$, and the accuracy of the correlation is typically $\pm 10\%$ as discussed by Hopkins and Inouye (1971).

The computed adiabatic wall temperature is $T_{aw}/T_\infty = 2.68$ which is within 3% of the theoretical value of $T_{aw}/T_\infty = 2.602$ obtained from the empirical formula

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

where $Pr_{tm} = 0.89$ is the mean turbulent Prandtl number.
In Fig. 20 the temperature-velocity relationship is evaluated. The data fit closely to the classical quadratic profile originally due to Wals (1969).

The log-linear plot of the mean streamwise velocity profile is shown in Fig. 21. The velocity is rescaled according to the Van-Driest transformation and the wall friction velocity. The height $y^+$ is in wall units. The logarithmic regions appears in the range $30 < y^+ < 150$. In this representation the velocity appears to be over-predicted when compared with the empirical and classical approximation $U_y / U_r = 2.5 \log(y^+) + 5.1$. The predicted profile fits more accurately with the equation $U_y / U_r = 2.9 \log(y^+) + 5.7$ (dashed line). In fact, the difference is not as large as it first appears. The representation is very sensitive with the exact friction velocity value ($y$ is measured in wall units, which is wall friction function). If $U_r$ is assumed to be equal to 0.0598 then the logarithmic region will fit perfectly with the classical equation. One explanation of this difference could be the inflow regeneration method that needs to be adjusted accurately (Lund et al. 1998). Further tests are in progress in order to evaluate the convergence of the constants 2.9 and 5.7 with mesh refinement as well.

Table 3  Flat Plate Boundary Layer Experimental Data

<table>
<thead>
<tr>
<th>Name</th>
<th>Mach No.</th>
<th>$Re_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES</td>
<td>3.0</td>
<td>$20 \times 10^3$</td>
</tr>
<tr>
<td>DNS Adams (1997)</td>
<td>3.0</td>
<td>$25 \times 10^3$</td>
</tr>
<tr>
<td>Johnson &amp; Rose (1975)</td>
<td>2.9</td>
<td>$1000 \times 10^3$</td>
</tr>
<tr>
<td>Konrad (1993)</td>
<td>2.0</td>
<td>$1590 \times 10^3$</td>
</tr>
<tr>
<td>Konrad &amp; Smits (1998)</td>
<td>2.87</td>
<td>$1900 \times 10^3$</td>
</tr>
<tr>
<td>Muck et al (1984, 1985)</td>
<td>2.87</td>
<td>$1638 \times 10^3$</td>
</tr>
<tr>
<td>Zheltovodov et al (1986)</td>
<td>1.7-9.4</td>
<td>up to $2000 \times 10^3$</td>
</tr>
</tbody>
</table>

All cases are adiabatic wall

The mean streamwise resolved turbulent kinematic normal stress $\langle u''u'' \rangle$, normalized using the local mean density $\langle \rho \rangle$ and wall shear stress $\tau_w$, is shown in Fig. 22. As discussed in Zheltovodov and Yakovlev (1986) and Smits and Duzaage (1996), the scaling $\langle \rho \rangle \langle u''u'' \rangle / \tau_w$ 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 Fig. 22 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 $M = 1.72 - 9.4$ 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 experimental Reynolds number. The decreasing slope corresponds precisely to Johnson and Rose (1975) data. For \(y/\delta < 0.2\) 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.

![Fig. 22 Reynolds normal stress](image1)

![Fig. 23 Reynolds shear stress](image2)

In Fig. 23 the 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.

**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 Yakovlev 1986, and Zheltovodov 1996) Reynolds-averaged Navier-Stokes simulations have failed to accurately predict the flow characteristics (Knight and Degre 1998) such as fluctuating pressure and heat transfer.

**Table 4 Compression Corner Experimental Data**

<table>
<thead>
<tr>
<th>Name</th>
<th>(\alpha)</th>
<th>Mach</th>
<th>(Re_5)</th>
<th>(Re_{e2})</th>
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<tr>
<td>LES</td>
<td>8(^{\circ})</td>
<td>3.0</td>
<td>(20 \times 10^3)</td>
<td>600</td>
</tr>
<tr>
<td>DNS Adams (1997)</td>
<td>18(^{\circ})</td>
<td>3.0</td>
<td>(25 \times 10^3)</td>
<td>n/a</td>
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<tr>
<td>Muck et al (1984)</td>
<td>8(^{\circ})</td>
<td>2.87</td>
<td>(1638 \times 10^3)</td>
<td>40800</td>
</tr>
<tr>
<td>Zheltovodov et al (1990)</td>
<td>8(^{\circ})</td>
<td>2.95</td>
<td>(75 \times 10^3)</td>
<td>2430</td>
</tr>
<tr>
<td>Zheltovodov et al (1990)</td>
<td>8(^{\circ})</td>
<td>2.8</td>
<td>(110 \times 10^3)</td>
<td>3950</td>
</tr>
</tbody>
</table>

All cases are adiabatic wall

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 8° compression corner at Mach 3.0 and $Re_x = 2 \times 10^4$ was performed. As indicated in Table 4, the configuration corresponds to the experiments of Zheltovodov and his colleagues except that the Reynolds number is lower for the LES. Table 4 also includes the flow conditions for other experiments and DNS which are references LES results.

The computational domain is $-6.0 \delta \leq x \leq 6.0 \delta$ where $\delta$ is the incoming boundary layer thickness and $x$ is measured from the corner (Fig. 24). The height and width of the computational domain are $L_y = 3.4 \delta$ and $L_x = 4.4 \delta$ (i.e., the same lengths as previous flat plate configuration). The grid is 1,600,000 tetrahedral cells. The nodal grid is stretched in the $y$ using a geometric factor of 1.088. The height $\Delta n$ of the first cell adjacent to the boundary is less than one wall unit.

Inflow data are extracted from the previous flat plate boundary layer LES (Fig. 18). At each time step, the velocity, pressure and temperature fields at the downstream station are rescaled and stored in a datafile. Storage is performed over a period equal to $3L_x/U_\infty$ (equivalent to $36\delta/U_\infty$), which yields about 14 GWords.

Fig. 24  Computational domain

Fig. 25  Shape factor

Fig. 26  Mean temperature vs velocity

Fig. 27  Mean wall pressure

Fig. 28  Mean wall pressure

The incompressible shape factor $H_f$ is displayed in Fig. 25 together with the corresponding result for the supersonic flat plate boundary layer. The initial evolution is identical as expected, indicating that the
upstream boundary is located sufficiently far from the corner to simulate an incoming equilibrium two dimensional turbulent boundary layer flow.

In Fig. 26 the temperature-velocity relationship is evaluated at different stations upstream and downstream of the shock. The simulation data fit well with the classical quadratic profile originally due to Walz (1969).

Fig. 27 displays the mean surface pressure on the wall. The value of $Re_x$ for the LES and the experiments of Zheltovodov are sufficiently close that the Reynolds number effect should not be significant, and therefore, since the mean flow is unseparated, scaling the distance $x$ by the boundary layer thickness $\delta$ is reasonable. Downstream of the shock, the value of the surface pressure reaches the level predicted by the experiments and inviscid theory. Additionally, the slope of the pressure rise seems to be correctly predicted.

A indirect check can be also be performed on the wall pressure. A compression corner at the same Mach number and Reynolds number but higher ramp angle $\alpha$ should provide a smoother pressure gradient, as observed experimentally (Zheltovodov et al 1990). The compression corner DNS from Adams (1997) uses the same Mach number, nearly the same Reynolds number, and a different corner angle $\alpha = 18^\circ$ (Table 4). Fig. 28 compares surface pressure along the wall. The data are here normalized with the downstream pressure level (maximum pressure) in order to take into account the difference in shock strength. The LES using $\alpha = 8^\circ$ effectively predicts a sharper slope than the DNS using $\alpha = 18^\circ$.

The mean velocity at $x/\delta = -3.3$ and $3.5$ is shown in Fig. 29. The computed profile displays close agreement with the experimental data of Zheltovodov et al. The decrease in velocity due to the shock is well reproduced in the computation except in the immediate vicinity of the wall where the difference between the computed
and experimental Reynolds number is likely to have an effect. The mean static temperature at \( z/\delta = -3.3 \) and 3.5 is shown in Fig. 30. The agreement between computation and experiment is very good.

The mean streamwise resolved turbulent kinematic normal stress \( \ll u''u'' \gg \), normalized using the local mean density \( \ll \rho \gg \) and upstream wall shear stress \( \tau_{wfl} \), is shown in Fig. 31. The reference wall shear stress is constant and measured at \( z = -2\delta \). Comparisons are presently shown with Muck et al (1984) \((\alpha = 8^\circ; M = 3; Re_\delta = 1.6 \times 10^6)\). In Fig. 32 the Reynolds shear stress distributions are shown for the same experiment. The deformation of these quantities associated with the unfavorable pressure gradient is evident in the vicinity of the corner. Their evolutions show a qualitative agreement. The Reynolds normal stress is amplified by a factor as high as 4. This maximum increase appears at \( y/\delta = 0.3 \), which is consistent with experiment. The similarity of the experimental data between \( 0.6 < y/\delta < 1.0 \) for different \( z \) is also evident in the LES. Similar tendencies and qualitative agreement with the computations are found with the Reynolds normal stress data of Zheltovodov and Yakovlev (1984, 1986), and Zheltovodov et al (1990). It is likely linked with the deformation of the large scale structures in the boundary layer. No conclusion can be drawn for the evolution of the typical peak in the near region due to its lack even in upstream experimental data. Essentially the same holds for the Reynolds shear stresses. Their amplifications correspond to experimental predictions.

![Figure 33](image1.png)  ![Figure 34](image2.png)

**Fig. 33** Instantaneous density at \( z = 2.2\delta \)  **Fig. 34** Instantaneous temperature at \( z = 2.2\delta \)

Figs. 33 and 34 show the instantaneous density and temperature contours within the boundary layer in an \( x - y \) plane. Large turbulent structures can clearly be seen, both upstream and downstream of the corner where the shock appears.
Bibliography


Personnel and Publications

Personnel

The personnel of the research project are listed in Table 5.

<table>
<thead>
<tr>
<th>Name</th>
<th>Title</th>
<th>Period of Participation</th>
<th>Supported by</th>
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<tr>
<td>Prof. Doyle Knight</td>
<td>Principal Investigator</td>
<td>1 Aug 96 - 30 Nov 98</td>
<td>this grant and Rutgers</td>
</tr>
<tr>
<td>Ms. Nora Okong'o</td>
<td>Graduate Assistant</td>
<td>1 Aug 96 - 30 Aug 98</td>
<td>this grant and Rutgers</td>
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<tr>
<td>Dr. Gerald Urbin</td>
<td>Postdoctoral Associate</td>
<td>16 Feb 98 - 30 Nov 98</td>
<td>this grant</td>
</tr>
<tr>
<td>Dr. Gang Zhou</td>
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<td>1 Jan 97 - 30 Sep 97</td>
<td>this grant</td>
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Papers


Papers Submitted


Visualization

