LES Modeling Errors in Free and Wall Bounded Compressible Shear Layers

Bernard Geurts, Bert Vreman, Hans Kuerten and Vassilios Theofilis

Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Abstract

We present direct numerical simulation results (DNS) for a compressible mixing layer and a compressible boundary layer on a flat plate in 2D. The exact filtered Navier-Stokes equations are derived and the contribution of the subgrid-terms and the discretisation errors is calculated by filtering the DNS data to a coarser grid. It will be shown that the discretisation errors are larger than the dominant subgrid terms if the filterwidth is comparable to the grid spacing. This holds for second and fourth order accurate spatial discretisations.

1 Introduction

Turbulent flow is generally believed to be well described by the Navier-Stokes equations. At sufficiently high Reynolds numbers the occurrence of small scale structures prevents a direct numerical simulation (DNS) of the equations, even in simple geometries. In order to predict flow properties at these high Reynolds numbers, one has to resort to a filtering of the equations. Adopting a filter operation which commutes with partial differentiation with respect to time and spatial coordinates one obtains the Large Eddy Simulation (LES) representation. In this filtering process new nonlinear quantities appear in the equations, e.g. averages of products of velocity components. Based on experimental evidence, intuition or mathematical convenience some of the new nonlinear terms are usually neglected, while others are modeled by relating these terms to filtered flow quantities. In order to solve the resulting filtered Navier-Stokes equations a discretisation in space and time is introduced. Hence, the types of errors occurring in the solution of the full Navier-Stokes equations in this approach may be classified as: disregard of several nonlinear terms (subgrid quantities), modeling errors in the Reynolds stresses and turbulent heat flow, and discretisation errors. It will be shown that in most compressible LES studies some important subgrid-terms are erroneously disregarded and that the discretisation error even dominates the terms that require modeling in case the filterwidth is comparable to the grid spacing.

We will consider a compressible mixing layer and a compressible boundary layer on a flat plate in order to obtain an appreciation of the various types of errors. In particular we filter DNS-results obtained for these flows to a coarser (LES) grid and calculate all the filtered terms arising from the Navier-Stokes equations as well as the discretisation errors. Typically, a four times coarser grid compared to the DNS grid is used as LES-grid. The time integration is performed with an explicit four stage Runge-Kutta method. The second order accurate spatial discretization is based on finite volumes with central spatial differencing [1]. The DNS-simulations and their 'LES-filtering' that will be presented are in two dimensions only. In the cases studied this corresponds to situations in which the energy spectrum is sharply decreasing (typically $\sim k^{-4}$), i.e. the contribution of the small scale structures is much smaller than in the corresponding 3D flows. This suggests that the relation between the discretisation error and the dominant subgrid terms certainly has to be considered in 3D LES studies. This will be subject of future investigations. The organisation of this paper is as follows. In section 2 we present the exact filtered Navier-Stokes equations. The compressible mixing layer is presented in section 3 and some results for the temporal flat plate flow are collected in section 4. We summarize our findings in section 5.

2 Filtering of the equations for compressible flow

The equations describing compressible flow are the well-known Navier-Stokes equations, which represent conservation of mass, momentum and energy:

$$\partial_t \rho = -\partial_j(\rho u_j), \quad (2.1)$$

$$\partial_t(\rho u_i) = -\partial_j(\rho u_i u_j) - \partial_i p + \partial_j \tau_{ij}, \quad (2.2)$$

$$\partial_t e = -\partial_j((e + p)u_j) + \partial_j(\tau_{ij}u_i) - \partial_j q_j. \quad (2.3)$$

Here the symbols ∂_t and ∂_j are abbreviations of the partial differential operators $\partial/\partial t$ and $\partial/\partial x_j$ respectively. The components of the velocity vector are denoted by u_i , while ρ is the density and p the pressure. Moreover, e is the total energy

$$e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u_i u_i. \quad (2.4)$$

The viscous stress tensor τ_{ij} is a function of temperature T and velocity vector $\mathbf{u}$, i.e. $\tau_{ij} \equiv F_{ij}(T, \mathbf{u})$ with

$$F_{ij}(T, \mathbf{u}) = \frac{\mu(T)}{Re} (\partial_j u_i + \partial_i u_j - \frac{2}{3} \delta_{ij} \partial_k u_k), \quad (2.5)$$

where $\mu(T)$ the dynamic viscosity, expressed by Sutherland's law for air,

$$\mu(T) = T^{\frac{3}{2}} \frac{1 + C}{T + C}. \quad (2.6)$$

In addition $q_j \equiv Q_j(T)$ represents the viscous heat flux vector, given by

$$Q_j(T) = -\frac{\mu(T)}{(\gamma-1)RePrM_R^2} \partial_j T. \quad (2.7)$$

Finally, the temperature T is related to the density and the pressure by the ideal gas law

$$T = \gamma M_R^2 \frac{p}{\rho}. \quad (2.8)$$

These equations have been made dimensionless by introducing a reference length L_R , a reference velocity u_R , a reference density ρ_R , a reference temperature T_R and a reference viscosity μ_R . In addition we set $\gamma = 1.4$, $Pr = 0.72$ and use $C = 110.4/T_R$. The values of the Reynolds number $Re = \rho_R u_R L / \mu_R$ and the reference Mach number $M_R = u_R / a_R$, where a_R is a reference value for the speed of sound, are given for each case separately.

Next we filter these equations. A filter operation extracts the large scale part $\bar{f}$ from a quantity f . In LES a spatial filter is employed,

$$\bar{f}(\mathbf{x}) = \int_{\Omega} G_{\Delta}(\mathbf{x} - \xi) f(\xi) d\xi, \quad (2.9)$$

where Ω is the flow domain and Δ denotes the filterwidth. The filtered equations that are presented here, are valid when the 'bar-filter' is any linear operator that commutes with the partial differential operators ∂_i and ∂_j . For compressible flow, Favre [2] introduced a related filter operation

$$\bar{f} = \frac{\overline{\rho f}}{\bar{\rho}}, \quad (2.10)$$

which in general does not commute with ∂_i and ∂_j .

When the bar-filter is applied to the continuity and momentum equations (2.1) and (2.2) we find

$$\partial_i \bar{\rho} = -\partial_j (\bar{\rho} \tilde{u}_j), \quad (2.11)$$

$$\begin{aligned} \partial_t (\bar{\rho} \tilde{u}_i) &= (-\partial_j (\bar{\rho} \tilde{u}_i \tilde{u}_j) - \partial_i \bar{p}) + [\partial_j \hat{\tau}_{ij} - \partial_j (\bar{\rho} a_{ij})] \\ &\quad + \{\partial_j (\bar{\tau}_{ij} - \hat{\tau}_{ij})\}, \end{aligned} \quad (2.12)$$

where $\hat{\tau}_{ij}$ is the stress tensor based on $\tilde{T}$ and $\tilde{\mathbf{u}}$, i.e. $\hat{\tau}_{ij} = F_{ij}(\tilde{T}, \tilde{\mathbf{u}})$. The quantity a_{ij} is the Reynolds stress tensor, defined as

$$a_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j. \quad (2.13)$$

In the filtered energy equation a modified total energy $\hat{e}$ is introduced, which is the total energy based on the filtered variables

$$\hat{e} = \frac{\bar{p}}{\gamma-1} + \frac{1}{2} \bar{\rho} \tilde{u}_k \tilde{u}_k = \bar{e} + \frac{1}{2} \bar{\rho} a_{kk}. \quad (2.14)$$

The $\hat{e}$ -equation is obtained when the bar-filter is applied to the energy equation (2.3) and the transport equation for the turbulent kinetic energy ($\bar{\rho}a_{kk}/2$) is subtracted. After a lengthy calculation one obtains

$$\begin{aligned} \partial_t \hat{e} = & -(\partial_j((\hat{e} + \bar{p})\tilde{u}_j)) \\ & + \left[\partial_j(\hat{\tau}_{ij}\tilde{u}_i) - \partial_j\hat{q}_j - \frac{1}{\gamma-1}\partial_j(\bar{p}\tilde{u}_j - \bar{p}\tilde{u}_j) - (\overline{p\partial_k u_k} - \bar{p}\partial_k \tilde{u}_k) - \partial_j(\bar{\rho}a_{kj}\tilde{u}_k) \right] \\ & + \left\{ \bar{\rho}a_{kj}\partial_j\tilde{u}_k + \overline{\tau_{kj}\partial_j u_k} - \bar{\tau}_{kj}\partial_j\tilde{u}_k + \partial_j(\bar{\tau}_{ij}\tilde{u}_i - \hat{\tau}_{ij}\tilde{u}_i) - \partial_j(\bar{q}_j - \hat{q}_j) \right\} \end{aligned} \quad (2.15)$$

in which the heat-flux $\hat{q}$ is based on the variable $\tilde{T}$, i.e. $\hat{q} = Q(\tilde{T})$.

We derived a system of filtered equations ((2.11), (2.12) and (2.15)) which is based on $(\bar{\rho}, \tilde{u}_j, \hat{e})$ as filtered flow quantities. This system of equations contains terms which can directly be identified with the unfiltered Navier-Stokes equations (2.1-3). Several additional nonlinear contributions (subgrid-terms) appear as well which cannot be directly related to the filtered flow quantities. If these equations are used as the basis for LES usually only the quantities a_{ij} and $\partial_j(\bar{p}\tilde{u}_j - \bar{p}\tilde{u}_j)$ are replaced by a model representation whereas the other nonlinear subgrid terms are simply disregarded. It is necessary to obtain an estimate of the order of magnitude of all these filtering errors in order to provide a more solid basis for turbulence modeling. We consider the results of direct numerical simulations of two simple flow problems: the compressible mixing layer and the compressible boundary layer on a flat plate.

3 The mixing layer

In this section the two dimensional temporal compressible mixing layer in a rectangular domain $[0...L_1, -L_2/2...L_2/2]$ is considered. Periodic boundary conditions are imposed in the x_1 -direction, and in the x_2 -direction the boundaries are free slip walls. The basic initial velocity profile is the hyperbolic tangent profile $U = \tanh(2x_2/\delta_{\omega,i})$, where $\delta_{\omega,i}$ is the initial value of the vorticity thickness [3]. We obtain the initial temperature profile from the Busemann-Crocco law [4] and the initial pressure distribution is uniform. The reference length L_R is half the initial vorticity thickness, while the reference density, velocity, temperature and dynamic viscosity are the initial upper stream values. A low amplitude perturbation consisting of a sinusoidal wave superimposed on uniform noise and multiplied with a Gaussian in the x_2 direction is initially added to the basic profile. The sinusoidal wave selected corresponds to the most unstable mode according to linear stability theory [5]. L_1 is set equal to twice the wave-length of the most unstable mode, i.e. so-called two-eddy simulations [3] are performed.

Direct numerical simulations are performed at $M_R = 0.2$ and $M_R = 0.6$ using $Re = 200$. The grid contains 256×256 cells. The simulations show the growth of the fundamental instability and the subsequent roll-up by which two vortices occur. These two vortices move towards each other and merge (Fig. 1). The simulations at $M_R = 0.2$ and $M_R = 0.6$ confirm the fact that an increased compressibility slows down the growth of the vorticity thickness (Fig. 2). The time at which the vorticity thickness attains its maximum value corresponds with the pairing of the vortices.

Figure 1: Vorticity at $t = 40$ (left) and $t = 120$ (right) at $M_R = 0.2$.

With the results of these direct numerical simulations the magnitude of the various terms, which were introduced in section 2, will be estimated. The data are filtered with the top-hat filter. The magnitude of all terms in the equations (2.12) and (2.15) is determined in the discrete L_2 -norm. First we consider the results of the $M_R = 0.2$ simulation and take the filterwidth Δ such that the support of the top-hat filter corresponds to 8×8 cells of the 256×256 grid. The filtered quantity is relatively smooth, since the filter width is much larger than the mesh distance. The partial derivative can be accurately approximated (relative error < 0.1 percent) using the fourth-order five point central difference. As an example of the magnitude and evolution of the filtered terms the norms $\|\partial_j \bar{\rho} a_{1j}\|$ and $\|\partial_j \hat{\tau}_{1j}\|$ are presented in Fig. 3. We notice that these two quantities, which are the Reynolds stress and the filtered viscous term in the x_1 -direction respectively, are of the same order of magnitude. The dotted curve in this figure shows the evolution of $\|\partial_j \bar{\rho} a_{1j}\|$ obtained from a direct simulation on a coarser 128×128 grid. We observe that the qualitative behavior is the same for these two simulations. This indicates that a resolution of 256×256 is adequate to investigate the effects in which we are interested here.

We will not present all filtered terms appearing in the equations as extensively as above. However, in order to obtain a rough appreciation of the orders of magnitude of the filtered terms we distinguish three classes: large (L), medium (M) and small (S). The various terms appearing on the right hand side of eqs. (2.12,15) have already been ordered such that the three groups of terms between brackets belong to (L), (M) and (S) respectively. First, we turn to the results at $M_R = 0.2$. Considering the momentum equation (2.12) the first two groups of terms are in (L) and (M) and the last in (S) with $(L) \approx 15(M) \approx 15000(S)$ in the L_2 -norm. In the $\hat{e}$ -equation the orders of magnitude are $(L) \approx 200(M) \approx 6000(S)$. At $M_R = 0.6$ the norms of the subgrid terms in class (M) are about two to three times smaller compared to $M_R = 0.2$. This illustrates the fact that the

Figure 2: Vorticity thickness δ_ω for $M_R = 0.2$ (solid) and $M_R = 0.6$ (dashed).

amount of turbulence in the mixing layer decreases when compressibility is increased. In this 2D flow a proper LES modeling should at least retain the large and medium terms, in particular the subgrid terms in class (M) are comparable in magnitude to the filtered viscous and heat flux terms. Specifically, it is observed that the pressure dilatation term ($\bar{p}\partial_k u_k - \bar{p}\partial_k \tilde{u}_k$) has to be modeled accurately, even at fairly low Mach numbers.

We next turn to the second type of errors, the numerical errors, that follow from the discretization on the coarse grid at which LES is performed. We introduce a coarse, uniform grid of 64×64 cells, with size h_i in the x_i direction. The approximation of the divergence operator ∂_j on this grid is denoted by δ_j . As a representative term, we consider the convective term $\partial_j(\bar{\rho} u_1 u_j)$. This term can be written as

$$\partial_j(\bar{\rho} u_1 u_j) - \delta_j(\bar{\rho} \tilde{u}_1 \tilde{u}_j) = \alpha + \beta \quad (3.1)$$

in which we introduced

$$\alpha = \partial_j \bar{\rho} a_{1j} ; \quad \beta = \delta_j(\bar{\rho} \tilde{u}_1 \tilde{u}_j) - \delta_j(\bar{\rho} \tilde{u}_1 \tilde{u}_j). \quad (3.2)$$

It is of interest to study the behavior of the subgrid term α and the discretisation error β as a function of the ratio r between the filter-width and the grid-spacing at constant h_i and variable Δ_i . An example of this behavior is obtained from the data at $M_R = 0.2$ and $t = 80$. Figure 4 presents $\|\alpha\|$, $\|\beta\|$ and $\|\alpha + \beta\|$ as functions of r . The discrete norm is based on the 64×64 grid and a second order finite volume discretization is applied. The proportionality of α with r^2 is readily observed. The application of a different filter with a square cosine kernel shows a similar relation. It has been proven for several filters, that the lowest order term in α is of order Δ^2 [6]. Figure 4 also shows that the discretization error β is larger than α , when $r \leq 2$. So the discretisation error is larger than the term that requires modeling. Hence, it does not make much sense to introduce a model for α in

Figure 3: Evolution of $\|\partial_j(\bar{\rho}a_{1j})\|$ (solid: 256×256 , dotted: 128×128) and $\|\partial_j\tau_{1,j}\|$ (dashed) at $M_R = 0.2$.

the case $\Delta_i = h_i$. Moreover, when r is increased, β only slowly decreases. The situation is improved if instead of the second order finite volume discretisation a five-point fourth order central difference scheme is used (Fig. 4). At $r = 1$ fourth order is equally bad but it clearly becomes superior when r is increased. This behavior is qualitatively independent of time after a transient originating from the initial white noise perturbation. During the transient the discretisation errors are even more dominant. The conclusion is that this type of LES-problem requires $\Delta_i > h_i$ and a fourth (or higher) order accurate spatial discretization of the convective terms.

4 The flat plate

In this section we consider the flow over a flat plate in two dimensions. We apply periodic boundary conditions in the streamwise (x_1) direction and use no-slip adiabatic conditions at the solid wall ($x_2 = 0$). In the far field we apply first order extrapolation of Riemann invariants. Moreover, we introduce a thin layer near the far field boundary in which we add low amplitude super-viscosity [3]. In this way outgoing waves are prevented from reflecting. The flow at $M_R = 0.5$ and $Re = 1000$, based on the displacement thickness δ^* , will be studied in detail. In order to prevent the flow to decay as an error-function profile in the long time regime we introduce a forcing term [7] driving the mean flow towards the solution of the compressible boundary layer equations. We first consider the validation of this approach in the linear regime by comparing the simulation results with predictions from linear stability theory. Then we present the results of the filtering procedure for this flow.

Linear stability theory gives rise to a generalized eigenvalue problem from which a prediction of the eigenvalues and corresponding eigenfunctions can be obtained [8, 9].

Figure 4: $\|\alpha\|$ (solid), $\|\beta\|$ (dashed) and $\|\alpha + \beta\|$ (dotted) obtained with a second order- (left) and a fourth order accurate discretisation (right) for the mixing layer.

Preparing an initial state consisting of the mean flow field superimposed upon a low amplitude perturbation allows for comparing the simulation results with the theoretical predictions, i.e. real (ω_r) and imaginary (ω_i) part of the eigenvalues and the corresponding eigensolution. The mean flow field is taken as the similarity solution of the compressible boundary-layer equations. A computational box with length $L_1 = 31$ was used in order to facilitate a comparison with literature [7]. The temporal eigenvalue corresponding to the most amplified eigensolution in this case is $\omega_r \approx 7.122 \times 10^{-2}$ and $\omega_i \approx 1.669 \times 10^{-3}$, in which we considered a constant dynamic viscosity μ . Two types of initial states are considered. First, a small perturbation consisting of the single most amplified eigensolution was studied. The fluctuating kinetic energy evolution initially exhibits linear growth at a rate equal to the imaginary part of eigenvalue corresponding to the solution selected and in the long time regime saturates due to nonlinear effects (see Fig. 5). A grid with 32×64 points stretched in the normal direction was used. Both real and imaginary parts of the eigenvalue compare to within 1 percent with the predictions of linear stability theory. Increasing the resolution results in an improved correspondence, e.g. at a resolution of 128×256 the errors are below 0.1 percent and are mainly due to uncertainties about extracting these values from the simulation data. These values agree much better with the theoretical predictions than those obtained in Ref. [7]. The second type of initial state consists of uniform noise superimposed on the mean field. Initially many individual eigenmodes are excited which are all stable except for one. Hence the evolution of the fluctuating kinetic energy initially shows a decrease, due to the fact that most modes contained in the initial state decay. After this transient only the most amplified mode remains and a similar linear growth is observed followed by a saturation (Fig. 5). The fluctuation in the streamwise velocity at a point close to the wall is also shown in Fig. 5. A clear 'purification' of the initially noisy signal corresponding to a decay of the stable

Figure 5: Fluctuating kinetic energy E (left) (solid: initial state with eigensolution perturbation, dashed: uniform noise perturbation) and streamwise velocity fluctuations u'_1 (right).

components in the signal and an exponential growth of the unstable mode is apparent. The fluctuations in the flow were found to correspond closely with the predicted eigensolution as well. These results show a good agreement with linear stability theory and serve as a validation of the numerical approach, including the treatment of the upper boundary condition.

We next consider the results obtained from filtering the simulation data corresponding to the initial state containing a uniform noise perturbation. The subgrid Reynolds stress α and the discretisation error β at $t = 3000$ are shown in Fig. 6. As in the mixing layer case these results are qualitatively independent of time after a transient of about 1500 time units. The simulation data obtained on a 128×64 stretched grid were interpolated with a local cubic polynomial fitting to a 128×256 uniform grid before the filtering was applied. We filtered the DNS data to a 32×64 grid. The results indicate that at low values of r both second and fourth order accurate schemes give rise to discretisation errors which are much larger than the subgrid Reynolds stresses themselves and as in the mixing layer flow a fourth order method is superior at larger r -values. Hence, these errors are of equal importance in wall bounded shear flows as in free shear flows in 2D.

5 Concluding Remarks

We have shown that the pressure dilatation term cannot be disregarded in LES-studies of compressible flow; its magnitude is comparable to the Reynolds stress and the viscous heat flux even at relatively low Mach numbers. Moreover, if the filterwidth is comparable to the grid-spacing an unacceptable discretisation error is observed, both in the mixing layer and in the flat plate flow. This holds for second and fourth order accurate spatial discretisation

Figure 6: $||\alpha||$ (solid), $||\beta||$ (dashed) and $||\alpha + \beta||$ (dotted) obtained with a second order- (left) and fourth order (right) accurate discretisation for the flat plate.

methods. A fourth order method becomes of use if the filterwidth is sufficiently larger than the grid spacing. In contrast, a second order method presents a large discretisation error in LES, even if the filterwidth is $\approx 4h$. A filtering of DNS data can also be used to compare various subgrid models. We have found e.g. that the well-known Smagorinsky model correlates poorly with the Reynolds stress a_{ij} . We will present detailed results of this study elsewhere.

References

- [1] J.G.M. Kuerten, B.J. Geurts, J.W. van der Burg, A.W. Vreman and P.J. Zandbergen, Proceedings ICNMF-conference, 1992.
- [2] Favre A., Physics of Fluids, **26**, 2851-2863, 1983.
- [3] Lesieur M., 'Turbulence in Fluids', Kluwer Academic Publishers, 1987.
- [4] F.M. White, 'Viscous Fluid Flow', McGraw-Hill, 1974.
- [5] W. Blumen, J.F.M, **40**, 769, 1970.
- [6] Germano M., Physics of Fluids, **29**, 1755-1757, 1986.
- [7] X. Normand and M. Lesieur, Theoret.Comput.Fl.Dyn, **3**, 231-252, 1992.
- [8] L.M. Mack, AGARD-Rep. No. 709, Lecture Series VKI, 1984.
- [9] M.R. Malik, NASA Rep. 3584, 1982.