ILES OF SHOCK WAVES AND TURBULENT MIXING USING HIGH-RESOLUTION RIEMANN SOLVERS AND TVD METHODS

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Abstract. This paper derives the implicit model for high-resolution MUSCL reconstruction-based upwind Godunov schemes for turbulent flows. A Mach number expansion of the numerical scheme allows analysis of the theoretical behaviour of the implicit subgrid model as the Mach number becomes small. This shows that different limiting methods within the same reconstruction technique have significantly different behaviour at low Mach numbers. For some methods the dissipation due to the Riemann solver dominates at low Mach, whereas for others the dominant terms are due to the averaging of the two limited quantities. Additionally it is shown that there are several terms which are identical in the implicit subgrid model as in the leading order of the Taylor series expansion of the large eddy simulations (LES) equations. Finally, results gained for three-dimensional shock-induced turbulent mixing of two different gases using the van Leer limiter is compared to the experimental results of Holder and Barton.

1 INTRODUCTION

This paper focuses on the analysis of high resolution Finite Volume Godunov methods for unsteady flows involving mixed compressible/incompressible regions. An example of this is the shock induced turbulent mixing of two different gases via Richtmyer-Meshkov (RM) type instabilities. This occurs when a shock wave passes through a perturbed interface between two gases, creating a turbulent mixing zone which grows in time. After the passage of the shock wave the RM instability is a low Mach number problem, depending, of course, on the initial conditions.

As the shock wave passes through the interface the upwind scheme provides the necessary dissipation to prevent overshoots, however once the shock has left the domain the turbulent flow field develops and kinetic energy is dissipated according to the truncation error of the numerical scheme. This dissipation is the ‘implicit’ dissipation embedded within the numerical scheme. In this paper the discretised equations are expanded in terms of Mach number and mesh size to...
Ben Thornber, Dimitris Drikakis examine the origin and form of the implicit dissipation for two limiting methods in a MUSCL framework. Through this analysis it is demonstrated that several leading order terms in the truncation error are identical to leading order terms computed by a Taylor series expansion of the LES equations. In addition it is illustrated that the order of the terms associated with the acoustic flux can differ significantly depending upon the limiter chosen. The applications of this analysis in the design of new limiters is also discussed.

2 Theoretical Analysis

In this paper it is assumed that the flow is inviscid and that the two gases have the same ratio of specific heats ($\gamma$), thus the governing equations reduce to the Euler equations. First the governing equations for a two dimensional system will be described in full. Next the theoretical expression for the Godunov flux is expanded in terms of Mach number, and simplified to the leading order terms for the two dimensional $\rho u$ momentum equation (extension to 3D and the other governing equations is straightforward). Finally, the reconstruction of the cell centred, cell averaged variables to the cell boundary is included within the analysis, and the expression truncated to give the leading order truncation error in terms of powers of Mach number, $\Delta x$ and $\Delta y$.

2.1 Governing Equations

The x-direction split two-dimensional Euler equations can be written as

$$\frac{\partial U}{\partial t} + A(U) \frac{\partial U}{\partial x} = 0,$$

where

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 0 & 0 \\ \hat{\gamma} V^2 - u^2 & (3 - \gamma) u & -\hat{\gamma} v & \hat{\gamma} \\ -uv & v & u & 0 \\ u ((\gamma - 3) V^2 - H) & H - \hat{\gamma} u^2 & -\hat{\gamma} uv & \gamma u \end{bmatrix},$$

$$H = \frac{E + p}{\rho} = \frac{a^2}{\hat{\gamma}} + V^2, \quad E = \rho V^2 + \rho e, \quad \rho e = \frac{p}{\hat{\gamma}}, \quad \hat{\gamma} = \gamma - 1, \quad V^2 = \frac{1}{2} (u^2 + v^2),$$

where $H$ is the total enthalpy; $E$ is the total energy; $u$ and $v$ are the velocity components; $\rho$ is the density. As this is a coupled hyperbolic system it possesses a set of real eigenvalues and linearly independent eigenvectors. The right eigenvectors $K$ can be employed to give the uncoupled characteristic form of the Euler equations

$$U = KW, \quad U_x = KW_x, \quad U_t = KW_t,$$

substitution into the Euler equations gives
\[ K \frac{\partial W}{\partial t} + AK \frac{\partial W}{\partial x} = 0, \]  

(5)
multiplication by \( K^{-1} \) gives a decoupled system of equations with respect to the characteristic variables \( W = K^{-1}U \)

\[ \frac{\partial W}{\partial t} + \Lambda \frac{\partial W}{\partial x} = 0, \]  

(6)
where \( \Lambda \) is the diagonal array of the eigenvalues \( \lambda \). For numerical purposes this diagonal array can be split into positive and negative parts given by

\[ \Lambda = \Lambda^+ + \Lambda^-, \quad |\Lambda| = \Lambda^+ - \Lambda^-. \]  

(7)

### 2.2 The Godunov Method at Low Mach Number

A basis of upwinding methods is to chose the upwind direction for each wave separately, thus mimicking the structure of the physical solutions of the governing equations. The Finite Volume fluxes for the Godunov method can be written in the following format\(^{10}\)

\[ F_{i+1/2} = \frac{1}{2} (F_L + F_R) - \frac{1}{2} |A| (U_R - U_L), \]  

(8)
where

\[ |A| = K |\Lambda| K^{-1}, \]  

(9)
where the subscripts \( R \) and \( L \) indicate the right and left side of the interface respectively. Note that \( |A| \) is not the same as the absolute of the Jacobian matrix \( \Lambda \). For the subsonic case the \( u \) and \( v \) velocities can be assumed subsonic and positive in the \( x \) direction, giving

\[ |\Lambda| = \begin{bmatrix} u & 0 & 0 & 0 \\ 0 & u & 0 & 0 \\ 0 & 0 & u+a & 0 \\ 0 & 0 & 0 & a-u \end{bmatrix}, \]  

(10)
and

\[ |A|_1 = \frac{1}{a^2} \begin{bmatrix} (a - u) (au + \hat{\gamma}V^2) \\ uI \\ v(\hat{\gamma}V^2 (a - u) - au^2) \\ J \end{bmatrix}, \]  

(11)
\[ |A|_2 = \frac{1}{a^2} \begin{bmatrix} u\hat{\gamma} (u - a) + au \\ a^2 + u^2 (\hat{\gamma}u - 2a\hat{\gamma} + a) \\ uv (\hat{\gamma}u - 2a\hat{\gamma} + a) \\ u (aH + \hat{\gamma}V^2 (u - a) - \hat{\gamma}au^2) \end{bmatrix}, \]  

(12)
\[ |A|_3 = \frac{1}{a^2} \begin{bmatrix} -v\hat{\gamma} (a-u) \\ uv\hat{\gamma} (u-2a) \\ a^2u + \hat{\gamma}v^2 (u-a) \\ v (L + a^2u) \end{bmatrix}, \quad |A|_4 = \frac{1}{a^2} \begin{bmatrix} \hat{\gamma} (a-u) \\ u\hat{\gamma} (2a-u) \\ \hat{\gamma} v (a-u) \\ -L \end{bmatrix}, \]

\[ I = a (au - a^2 - u^2) + \hat{\gamma} V^2 (2a - u), \]

\[ J = (a^2 (a + u) + \hat{\gamma} V^2 (a - u) + au^2 (\gamma - 2)) V^2 - a^3 \gamma u^2 / \hat{\gamma} - a^2 uv^2, \]

\[ L = -a^3 + \hat{\gamma} V^2 (u - a) - a \hat{\gamma} u^2, \]

where \[ |A|_1 \] indicates column 1 of the matrix \[ |A| \] and \( a \) is the speed of sound. As can be seen this is a complex expression. Equations (12) to (16) can be simplified by assuming the case where the flow is nearly incompressible as is the case once the shock wave has left the domain of interest. Next the variables are non-dimensionalised by a reference quantity which is the maximum value of the variable within the domain, and expanded in terms of Mach number as follows

\[ \rho = \rho_{ref} \left( \rho_0 + M^2 \rho_2 + ... \right) \]

\[ u = a_{ref} \left( 0 + Mu_1 + ... \right) \]

\[ v = a_{ref} \left( 0 + Mv_1 + ... \right) \]

\[ p = \rho_{ref} a_{ref}^2 \left( p_0 + M^2 p_2 + ... \right), \]

giving to first order in \( M \)

\[ |A|_{M<<1} \approx \begin{bmatrix} Ma_{ref}u_1 & Mu_1 (2 - \gamma) / a_0 & -Mv_1 \hat{\gamma} / a_0 & \hat{\gamma} / a_{ref} a_0 \\
-Mu_1 a_{ref}^2 a_0 & a_{ref} a_0 & 0 & 2M u_1 \hat{\gamma} / a_0 \\
0 & 0 & Ma_{ref} u_1 / a_0 & \hat{\gamma} M v_1 / a_0 \\
0 & Ma_{ref}^2 u_1 / \hat{\gamma} & -Ma_{ref}^2 v_1 / a_0 & a_{ref} a_0 \end{bmatrix}, \]

also,

\[ \begin{bmatrix} \Delta \rho \\ \Delta \rho u \\ \Delta \rho v \\ \Delta E \end{bmatrix} \approx \begin{bmatrix} \rho_{ref} \Delta \rho_0 \\ \rho_{ref} a_{ref} \Delta (\rho_0 u_1) \\ \rho_{ref} a_{ref} \Delta (\rho_0 v_1) \\ \rho_{ref} a_{ref}^2 \Delta (\rho_0) \end{bmatrix}, \]

and,

\[ \rho u^2 \approx M^2 \rho_{ref} a_{ref}^2 \rho_0 u_1^2 \]

\[ \rho uv \approx M^2 \rho_{ref} a_{ref}^2 \rho_0 u_1 v_1 \]

\[ p \approx \rho_{ref} a_{ref}^2 \rho_0. \]
Inserting this into equation (8) for the x-split momentum equation, and only retaining the leading order terms for the Riemann solver

\[
(\rho u^2 + p)_{i+1/2} = \frac{1}{2} \left( (M^2 \rho_0 u_1^2 + p_0)_{L,i+1/2} + (M^2 \rho_0 u_1^2 + p_0)_{R,i+1/2} \right) \\
- \frac{M}{2} \left( \rho_0 a_0 \Delta_{i+1/2} u_1 + 2 u_1 \hat{\gamma} \Delta_{i+1/2} (p_0) / a_0 \right). \tag{26}
\]

This dependance of the numerical dissipation on the Mach number of the flow is well known, and is the reason why preconditioning of the compressible equations is required to gain accurate results for very low mach number flows. 2, 3 The notation \(\Delta_{i+1/2}\) has been introduced as a difference over the \(i+1/2\) interface. The terms in \(M^2\) from \(|A|\) have been neglected as they are multiplied by at least \(\Delta x^2\) for a second order scheme in space thus making them relatively small.

For the y-direction split equations there is also a contribution to the \(\rho u\) momentum equations for flux of \(\rho u\) out of the y direction faces. This is of the form

\[
(\rho u v + p)_{j+1/2} = \frac{1}{2} \left( (M^2 \rho_0 u_1 v_1 + p_0)_{L,j+1/2} + (M^2 \rho_0 u_1 v_1 + p_0)_{R,j+1/2} \right) \\
- \frac{M}{2} u_1 \hat{\gamma} \Delta_{j+1/2} (p_0) / a_0. \tag{27}
\]

2.3 Truncation Error of the Discretised Equations

Given the fluxes at the interfaces, the total flux can be written as

\[
F_{1,j} = \frac{F_{i+1/2,j} - F_{i-1/2,j}}{\Delta x} + \frac{F_{i,j+1/2} - F_{i,j-1/2}}{\Delta y} \tag{28}
\]

where \(\Delta x\) and \(\Delta y\) are the cell length and height respectively, and are non-dimensionalised by a characteristic length scale of the flow. Considering only the fluxes at interfaces \(i+1/2\) and \(j+1/2\), the flux for the u-momentum equation can be written as

\[
F_{\rho u} = F_{av} - F_{RS} \tag{29}
\]

\[
F_{av} = \frac{1}{2} \frac{\partial}{\partial x} \left( (M^2 \rho_0 u_1^2 + p_0)_{L,i+1/2} + (M^2 \rho_0 u_1^2 + p_0)_{R,i+1/2} \right) + \frac{1}{2} \frac{\partial}{\partial y} \left( (M^2 \rho_0 u_1 v_1 + p_0)_{L,j+1/2} + (M^2 \rho_0 u_1 v_1 + p_0)_{R,j+1/2} \right), \tag{30}
\]

\[
F_{RS} = \frac{M}{2} \frac{\partial}{\partial x} \left( \rho_0 a_0 \Delta_{i+1/2} u_1 + 2 u_1 \hat{\gamma} \Delta_{i+1/2} (p_0) / a_0 \right) + \frac{M}{2} \frac{\partial}{\partial y} u_1 \hat{\gamma} \Delta_{j+1/2} (p_0) / a_0, \tag{31}
\]
where $F_{av}$ represents the average of the fluxes computed from the left and right states, and $F_{RS}$ is the correction due to the Riemann solver. Therefore the contribution of the Riemann solver is proportional to the difference between the two limited quantities multiplied by the Mach number, i.e. a function of both Mach number and the cell dimensions. The reason for this is that the wave jumps at the interface will be decreased with increasing grid resolution, thus decreasing the strength of the resulting acoustic fluxes.

It is well known that the behaviour of a numerical scheme can be determined via examination of the truncation error. The truncation error of a scheme is derived by expanding the discretised equations as a Taylor series in powers of $\Delta x$ and $\Delta y$ with respect to the cell centred, cell averaged variables. Equation (29) gives an explicit form for determination of the implicit subgrid terms which dissipate turbulent kinetic energy. This paper focuses on the MUSCL reconstruction scheme, where the boundary extrapolated variables are given by

$$U_{i+1/2}^L = U_i + \frac{1}{4} \left[ (1 - k) \phi (r^L) (U_i - U_{i-1}) + (1 + k) \phi \left( \frac{1}{r^L} \right) (U_{i+1} - U_i) \right],$$  \hspace{1cm} (32)$$

$$U_{i+1/2}^R = U_{i+1} - \frac{1}{4} \left[ (1 - k) \phi (r^R) (U_{i+2} - U_{i+1}) + (1 + k) \phi \left( \frac{1}{r^R} \right) (U_{i+1} - U_i) \right],$$  \hspace{1cm} (33)

where,

$$r^L = \frac{U_{i+1} - U_i}{U_i - U_{i-1}},$$  \hspace{1cm} (34)$$

$$r^R = \frac{U_{i+1} - U_i}{U_{i+2} - U_i}.$$  \hspace{1cm} (35)

Two limiters functions $\phi$ of general interest are defined away from extrema as

$$\phi_{VL} = \frac{2r}{1 + r},$$  \hspace{1cm} (36)$$

$$\phi_{MM} = \min (1, r).$$  \hspace{1cm} (37)

where VL indicates van Leer and MM is Minmod. The implicit model for each of these limiters is defined as the exact Taylor series expansion minus the approximate solution. Using symbolic manipulation software such as Mathematica, an explicit expression for these terms can be gained. From this point the subscripts referring to the Mach number expansion of the flow variables will not be included for clarity. Defining

$$TE_{AV} = \frac{\partial}{\partial x} \left( \rho u^2 + p \right)_{i+1/2} + \frac{\partial}{\partial y} (\rho u v) - F_{AV},$$  \hspace{1cm} (38)$$

$$TE_{RS} = F_{RS},$$  \hspace{1cm} (39)
the truncation errors are
\[ T_{AV}^{VL} = \frac{\Delta x^2}{12} \frac{\partial}{\partial x} \left( 2M^2 u_{xx} + p_{xx} \right) + M^2 \Delta y^2 \frac{\partial}{\partial y} \left( u_{yy} + u_{yy} v \right), \]  

(40)

where \( (\cdot)_x = \partial / \partial x \). Surprisingly, the Minmod limiter also gives this form for \( T_{AV} \). Next, examining the contributions from the Riemann solver

\[ T_{RS}^{VL} = M \Delta x^3 \frac{\partial}{\partial x} \left( \rho a \left| u_{xx} \right| u_x - u_{xxx} \right) + \frac{2u^\gamma}{a} \left[ \frac{p_{xx}}{p_x} - p_{xxx} \right] + \frac{M}{4} \frac{\Delta y}{a} \frac{u^\gamma}{\partial y} \left| \frac{p_{yy}}{p_y} - p_{yyy} \right|, \]  

(41)

\[ T_{RS}^{MM} = M \Delta x^2 \frac{\partial}{\partial x} \left( \rho a \left| u_{xx} \right| u_x + \frac{2u^\gamma}{a} \left| \frac{p_{xx}}{p_x} \right| \frac{p_x}{p} \right) + M \frac{\Delta y^2}{4} \frac{u^\gamma}{a} \frac{\partial}{\partial y} \left| \frac{p_{yy}}{p_y} \right| p_y. \]  

(42)

### 2.4 Discussion

For the van Leer limiter it can be seen that as long as the mesh is sufficiently fine compared to the Mach number, i.e. \( \Delta x \ll M \) then the truncation error is dominated by \( T_{AV} \). This assumption cannot be made for the Minmod limiter, as \( T_{RS} \propto M \Delta x^2 \), which in subsonic flows would always be larger than the contribution of \( T_{AV} \propto M^2 \Delta x^2 \). This is also true of several other limiters, see Thornber and Drikakis\(^9\) for example.

Ideally the truncation errors given by equations (40) to (42) would exactly match the Taylor series expansion of the subgrid stresses in terms of the cell averaged flow variables. The LES equations can be expanded in a Taylor series (as done for LES models based on approximate deconvolution) to give the subgrid velocities as a function of the cell averaged quantities. To leading order the resultant terms are\(^5,8\)

\[ T_{Ideal} = \frac{\Delta x^2}{12} \left[ M^2 (u_x u_x)_x + M^2 (u_x v_y)_y + \frac{p_{xxx}}{2} \right] + M^2 \frac{\Delta y^2}{12} \left[ (u_y u_y)_x + (u_y v_y)_y \right]. \]  

(43)

Assuming that \( \Delta x \ll M \), equations (43) and (40) can be directly compared. Firstly it can be seen that the both the ideal and actual truncation errors are of second order accuracy. It is also clear that several terms are identical, these are

\[ \frac{\Delta x^2}{6} M^2 u_x u_{xx}, \quad \frac{\Delta y^2}{12} M^2 (u_y v_{yy} + u_{yy} v_y). \]  

(44)

Also the pressure term \( p_{xxx} \) is present in both, however there is a factor of \( 1/24 \) in the cell averaged Euler equations compared to \( 1/12 \) in the truncation error. There are some terms not present in the truncation error, notably the cross-derivatives (which may not have a strong
effect\(^5\)). This is due to the one dimensional nature of the variable extrapolation, and could be improved by using two-dimensional stencils. Finally the truncation error has additional terms of a hyperviscosity form

\[
\frac{\Delta x^2}{6} M^2 u_{xxx}, \quad \frac{\Delta y^2}{12} M^2 (u_{yyy} + u_{ygyg}).
\] (45)

This analysis suggests that in the design for ILES methods used in mixed compressible/incompressible flows it would be useful to derive limiters which have a second order accuracy but that the leading order difference between the left and right interpolated values be much higher. This would reduce the influence of the dissipation of the Riemann solver, thus giving dominance to the terms which are identical in both the ideal expansion and truncation errors.

In a near-incompressible turbulent flow field it is possible that Riemann-type dissipation would be undesirable at scales at least some way into the sub-inertial range. If this is the case, then, as the Mach number of eddies decreases with size, the criteria \(\Delta x << M\) could become restrictive.

3 Half Height Experiment

The half height experiment of Holder and Barton\(^4\) is simulated to illustrate the performance of the van Leer limiter in complex flows involving shock waves and turbulent mixing. In this experiment a shock of Mach = 1.26 is passed through a block of SF\(_6\). As it passes through the block, the shock wave slows causing a Kelvin-Helmholtz type shear layer at the upper interface of the block, with Richtmyer-Meshkov mixing at the vertical interfaces. The shock then reflects off the back wall, passing back through the mixing zone, and down the shock tube. A schematic of the experiment is shown in Figure 1.

![Figure 1: Schematic of the half height experiment](image)

The governing equations used for the simulation are the five Euler equations plus two equations modelling the gas mixture. The two additional equations are from the multi-component
A characteristics based Riemann solver has been derived for this system of equations following the method used by Eberle. Higher order of accuracy was achieved using the MUSCL scheme with the van Leer limiter, and it has been implemented in a CFD code called CNS3D developed by the authors. The mesh size was $600 \times 160 \times 320$, with periodic y-direction boundary conditions. In addition, a random perturbation of RMS amplitude 0.1mm was added to the vertical interfaces. The drain hole is not modelled.

At the latest time the typical Mach number of the primary vortex is 0.1, and the mesh size $\Delta x = 6.25 \times 10^{-4}$, where $\Delta x$ is non-dimensionalised by the size of the primary vortex. Thus it can be assumed that the truncation errors $T_{AV}$ in equation (40) dominate. This means that several of the exact leading order terms that represent the large eddy filtering process are represented exactly by the truncation error of the scheme in smooth areas of flow.

Figure 2 shows iso-surfaces of constant volume fraction at $t = 4\text{ms}$.
Figure 3: Comparison of experimental images (left, © British Crown Copyright 2006/MOD) and mass of SF$_6$ density (kg/m$^3$) for CNS3D with MUSCL and van Leer limiting (right)
and simulation. This indicates that the growth of the large scales, i.e. the main vortex, is well represented. Finally at 4ms it can be seen that there is a discrepancy in the direction of the mushroom shaped perturbation. In the simulation, a series of reflected shock waves induce an upward velocity, thus the mushroom points upwards. It is believed that in the experiment these shock waves pass through the drainhole and so the mushroom remains horizontal.

In summary, good agreement is gained throughout the duration of the experiment, considering the initial modelling assumptions.

4 CONCLUSIONS

The above theoretical analysis points to better performance of the van Leer limiter at low Mach number due to the reduced influence of the Riemann solver compared to Minmod. It also demonstrates a clear and exact link between several terms in the truncation error of the MUSCL schemes, and the Taylor series expansion of the LES equations, assuming that the criteria \( \Delta x \ll M \) is satisfied. Finally it suggests designing a class of limiters of second order accuracy where the difference between the left and right limited quantity is of third or higher order.

The van Leer limiter was employed to simulate turbulent mixing of two different gases. The results gained compare favourably with experiment in terms of shock position (validating the multi-component model) and growth of the dominant length scales.

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