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Numerical dissipation of upwind schemes in low Mach flow

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SUMMARY

This paper presents a modified Roe scheme for the simulation of multicomponent compressible flows with low Mach features. This modification reduces the excess dissipation of kinetic energy in Godunov-type methods at low Mach. The modification is shown to work effectively to $Ma = 0.0002$ using a single-mode Kelvin–Helmholtz instability as a test case, and reproduces the correct Ma^2 incompressible pressure scaling. Computational expense is negligible. Copyright © 2007 John Wiley & Sons, Ltd.

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KEY WORDS: Godunov; upwind; multicomponent; low Mach; Roe

1. INTRODUCTION

It is quite common to use Godunov-type upwind methods for simulation of flows with both compressible and incompressible nature, or where the monotonicity of certain properties are required. An example of this is the Richtmyer–Meshkov instability, where a shock wave passes through a perturbed interface, generating a turbulent mixing layer. Once the shock wave has passed, the mixing layer develops in a largely incompressible manner. It is well known that upwind schemes are excessively dissipative at low Mach number; however, the mechanism for this is not widely understood. A recent analysis [1] shows that the increase in entropy is approximately equal to the irreversible dissipation of kinetic energy at low Mach. It also shows that the leading order increase of entropy in Godunov-type methods is due to numerical dissipation within the momentum

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equations, which can be written as

$$T\Delta S=\varepsilon_{\mathrm{num}}=\frac{(1-\mathscr{C})}{4\Delta x}a\Delta u^2+\cdots \tag{1}$$

where T, u and a are the temperature, velocity normal to the cell interface and speed of sound, respectively. Δx is the length of the computational cell, $\mathscr{C}$ the Courant–Friedrich–Levy (CFL) number, ΔS the change in entropy. $\varepsilon_{\mathrm{num}}$ is the numerical dissipation of kinetic energy. It can be seen that the dissipation rate becomes infinite as $Ma\rightarrow 0$ (equivalently as $a\rightarrow\infty$). This paper derives a new Roe scheme for the multicomponent equation set of Wang *et al*. [2] and proposes a modification of the numerical dissipation in the momentum equations which corrects the Mach number dependence of the numerical dissipation. The performance of this scheme is illustrated *via* a simple single-mode Kelvin–Helmholtz (KH) test case.

2. GOVERNING EQUATIONS AND NUMERICAL SCHEME

This paper concerns the low Mach performance of compressible, multicomponent schemes. The governing equations chosen are the Euler equations plus two additional equations for the multi-component model. The three-dimensional compressible Euler equations for a Cartesian co-ordinate system can be written in conservative variables as

$$\frac{\partial\mathbf{U}}{\partial t}+\frac{\partial\mathbf{E}}{\partial x}+\frac{\partial\mathbf{F}}{\partial y}+\frac{\partial\mathbf{G}}{\partial z}=0 \tag{2}$$

where

$$\mathbf{U}=[\rho,\ \rho u,\ \rho v,\ \rho w,\ e]^{\mathrm{T}},\quad \mathbf{E}=[\rho u,\ \rho u^2+p,\ \rho uv,\ \rho uw,\ \ (e+p)u]^{\mathrm{T}}$$

$$\mathbf{F}=[\rho v,\ \rho uv,\ \rho v^2+p,\ \rho vw,\ (e+p)v]^{\mathrm{T}},\quad \mathbf{G}=[\rho w,\ \rho uw,\ \rho vw,\ \rho w^2+p,\ (e+p)w]^{\mathrm{T}}$$

$$e=\rho i+0.5\rho q^2$$

where ρ, i, u, v, w are the density, internal energy and Cartesian velocity components, respectively. The system of equations is completed with the specification of an ideal gas equation of state, $p=\rho i(\gamma-1)$. The multi-component model employed is that proposed by Wang *et al.* [2], which is based on the conservation of total enthalpy within the fluid mixture and consists of tracking two additional equations

$$\frac{\partial}{\partial t}\left(\frac{\rho\chi}{M}\right)+\frac{\partial}{\partial x}\left(\frac{\rho u\chi}{M}\right)+\frac{\partial}{\partial y}\left(\frac{\rho v\chi}{M}\right)+\frac{\partial}{\partial z}\left(\frac{\rho w\chi}{M}\right)=0 \tag{3}$$

$$\frac{\partial}{\partial t}\left(\frac{\rho}{M}\right)+\frac{\partial}{\partial x}\left(\frac{\rho u}{M}\right)+\frac{\partial}{\partial y}\left(\frac{\rho v}{M}\right)+\frac{\partial}{\partial z}\left(\frac{\rho w}{M}\right)=0 \tag{4}$$

where M is the molecular mass of the mixture, and the variable $\chi=\gamma/(\gamma-1)$ for a perfect gas. A new Roe scheme has been derived for this set of governing equations, solved in a direction-split form. The flux for the Roe scheme can be written as

$$\mathbf{F}_{i+1/2}=\frac{1}{2}(\mathbf{F}_L+\mathbf{F}_R)-\frac{1}{2}\sum_{i=1,7}\alpha_i|\lambda_i|\mathbf{K}^i \tag{5}$$

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where the eigenvalues are

$$\lambda_1=\lambda_2=\lambda_3=\lambda_4=\lambda_5=u, \quad \lambda_6=u-a, \quad \lambda_7=u+a \tag{6}$$

and the speed of sound $a^2=(H-\frac{1}{2}V^2)/(\chi-1)$. With some algebraic manipulation the eigenvectors can be cast into the following form:

$$K^1=\begin{bmatrix}0\\0\\0\\0\\0\\\chi\\1\end{bmatrix}, \quad K^2=\begin{bmatrix}0\\0\\0\\0\\-a^2(\chi-1)M/\chi\\-1\\0\end{bmatrix}, \quad K^3=\begin{bmatrix}1\\u\\v\\w\\V^2/2\\0\\0\end{bmatrix}, \quad K^4=\begin{bmatrix}0\\0\\1\\0\\v\\0\\0\end{bmatrix} \tag{7}$$

$$K^5=\begin{bmatrix}0\\0\\0\\1\\w\\0\\0\end{bmatrix}, \quad K^6=\begin{bmatrix}1\\u-a\\v\\w\\a^2(\chi-1)-au+\frac{1}{2}V^2\\\chi/M\\1/M\end{bmatrix}, \quad K^7=\begin{bmatrix}1\\u+a\\v\\w\\a^2(\chi-1)+au+V^2/2\\\chi/M\\1/M\end{bmatrix} \tag{8}$$

The wave strengths, α_i, required for the Roe scheme are given by

$$\alpha_1=\frac{\Delta u_6}{\chi}-\frac{2}{M}\overline{\Delta A}, \quad \alpha_2=\chi\overline{\Delta u_7}, \quad \alpha_3=-M\overline{\Delta u_7}+\Delta u_1-2\overline{\Delta A}, \quad \alpha_4=\Delta u_3-v\Delta u_1$$

$$\alpha_5=\Delta u_4-w\Delta u_1, \quad \alpha_6=M\overline{\Delta u_7}/2-(\Delta u_2-u\Delta u_1)/2a+\overline{\Delta A}$$

$$\alpha_7=\alpha_6+(\Delta u_2-u\Delta u_1)/a$$

$$\overline{\Delta A}=\frac{\Delta u_5-u\Delta u_2-v\Delta u_3-w\Delta u_4+\frac{1}{2}V^2\Delta u_1}{2a^2(\chi-1)}, \quad \overline{\Delta u_7}=\Delta u_7-\frac{1}{\chi}\Delta u_6 \tag{9}$$

Following the analysis by Guillard and Viozat [3] the asymptotic behaviour of dissipation in the Roe flux can be determined. This is achieved by substituting

$$\begin{aligned}
\rho &= \rho_{\text{ref}}(\rho_0+Ma^2\rho_2+\cdots), \quad u=a_{\text{ref}}(0+Ma\,u_1+\cdots)\\
v &= a_{\text{ref}}(0+Ma\,v_1+\cdots), \quad w=a_{\text{ref}}(0+Ma\,w_1+\cdots)\\
p &= \rho_{\text{ref}}a_{\text{ref}}^2(p_0+Ma^2p_2+\cdots)
\end{aligned} \tag{10}$$

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into Equation (5), where Ma is the reference Mach number. Next all terms (for all equations) in the computation of the Roe flux are expanded to leading order in Mach. There is only one leading order term at low Mach, giving

$$(\rho u^2+p)_{i+1/2} \approx \tfrac{1}{2}((\rho u^2+p)_L+(\rho u^2+p)_R)+\tfrac{1}{4} Ma\, \rho_{\mathrm{ref}} a_{\mathrm{ref}}^2 a_0(\Delta(\rho_0 u_1)-u_1\Delta(\rho_0)) \tag{11}$$

This single term is the only term of order Mach, and arises because $\alpha_6=-\alpha_7$ and, $K_2^6=-K_2^7$, where $(\cdot)_2$ indicates the second row of the eigenvector. As expected, this result is identical to that given in the analysis of the Euler equations under Godunov form [4] (noting that $\Delta(\rho_0 u_1)-u_1\Delta(\rho_0)=\rho_0\Delta(u_1)$). The next terms in the expansion are constant with Mach; hence, these are not the source of increased dissipation in incompressible flows and are neglected here. Computing the dissipation of kinetic energy due to this term gives the leading order term shown in Equation (1). As $Ma\to 0$ ($a_{\mathrm{ref}}\to\infty$) then the Roe scheme gives infinite dissipation. To rectify this, one can modify the second row of the eigenvectors K_2^6 and K_2^7 by a factor of Mach in low Mach regions. In this paper the sixth and seventh eigenvectors are modified as

$$K_2^6=u-a\to u-\beta a, \quad K_2^7=u+a\to u+\beta a \tag{12}$$

Here, $\beta=\min(10Ma, 1)$, such that the original Roe scheme is recovered for interfaces where $Ma>0.1$. This makes the leading order dissipation tend to a constant value as Mach tends to zero. If the new flux Jacobian is computed using the new set of eigenvectors it is seen that this modification changes only the u-momentum flux from ρu^2+p to $\rho u^2+\beta p$. The modification could be viewed as a change in the governing equations that are being solved, which is not desirable. However, the standard fluxes are dominated by unphysical viscous dissipation at low Mach, and are hence also not solving the Euler equations—but the Euler equations plus a large viscous term. The contribution from the Roe scheme can be understood as an additional term required only to stabilize the central difference flux. Hence, the form of this stabilization does not necessarily require a physical basis, but it must not dominate the flow physics (as happens with the standard flux at low Mach). This modification also allows good stability according to the standard CFL condition, as opposed to standard preconditioned methods where stability in explicit time stepping is prohibitive [5], thus can be used where the time stepping is not constrained by the low Mach portion of the flow. In addition, it preserves exactly a stationary material interface.

3. NUMERICAL TEST CASES

The effective resolution of the modified Roe scheme is now tested in the simulation of a single-mode KH instability. The above method is implemented in conjuction with third-order accurate Runge–Kutta time stepping [6], and with fifth-order (in one dimension) MUSCL reconstruction [7]. The computational domain is square and spans $[-0.5,-0.5]$ to $[0.5, 0.5]$ and is discretized with 16 cells in each direction. The initial conditions consist of a perturbed shear layer, where the flow is initially parallel, but for a small perturbation velocity which triggers the development of a KH vortex. The initial perturbation is written in the form of the divergence of a vector potential

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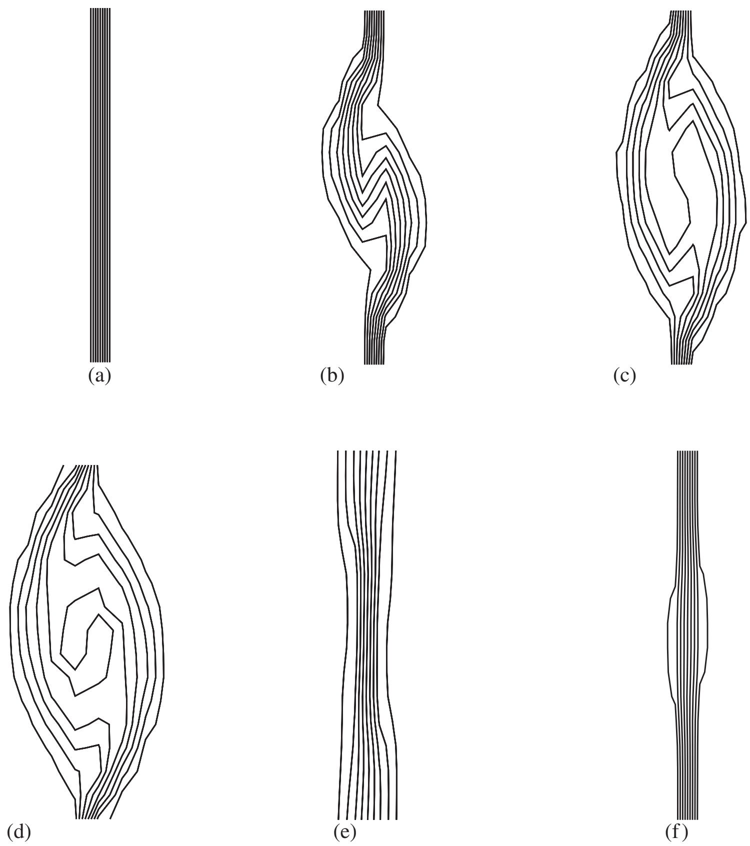

Figure 1. Time development of the single-mode KH instability using the standard Roe scheme. Nine contours of volume fraction from 0.1 to 0.9: (a) $t=0$, $Ma=0.2$; (b) $t=1$, $Ma=0.2$; (c) $t=2$, $Ma=0.2$; (d) $t=3$, $Ma=0.2$; (e) $t=3$, $Ma=0.02$; and (f) $t=3$, $Ma=0.002$.

A_z so that the flow field is approximately solenoidal [8]. In summary,

$$
\begin{aligned}
v &= -\Delta V/2 - \frac{\partial A_z}{\partial x}, \quad u = \frac{\partial A_z}{\partial y} \text{ for } x<0 \\
v &= \Delta V/2 + \frac{\partial A_z}{\partial x}, \quad u = \frac{\partial A_z}{\partial y} \text{ for } x>0 \\
A_z &= \frac{V_0}{k}\cos(ky)\exp^{-k|x|}, \quad V_0 = 0.1\Delta V, \ \ \Delta V = 1
\end{aligned} \tag{13}
$$

where ΔV is the difference in mean flow velocity V across the mixing layer. The Mach number, defined by $\Delta V/a$, is adjusted by changing the pressure. Density is fixed at $\rho=1$, and $\gamma=\frac{5}{3}$. The coarse resolution is deliberately chosen to highlight the scheme's ability to capture what would be a high wavenumber perturbation on a larger grid. It also allows easy demonstration of the low Mach behaviour of the dissipation of kinetic energy.

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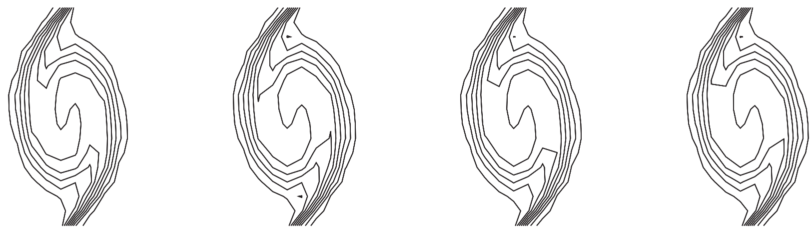

Figure 2. Nine contours of volume fraction from 0.1 to 0.9 at $t=3$ for the modified scheme: (a) $Ma=0.2$; (b) $Ma=0.02$; (c) $Ma=0.002$; and (d) $Ma=0.0002$.

Table I. Scaling of the maximum pressure and density fluctuations with Mach at $t=3$.

Mach (Ma)	$\Delta p_{\max}/(p Ma^2)$	$\Delta \rho_{\max}/(\rho Ma^2)$
0.2	0.683	0.525
0.02	0.633	0.575
0.002	0.650	0.35
0.0002	0.633	12.5

The development of the instability when using the standard Roe scheme at $Ma=0.2$ is illustrated in Figure 1(a)–(d). The initially small perturbation is absolutely unstable and forms the characteristic KH vortex. Contours of volume fraction are also shown in Figure 1(e) and (f) for $Ma=0.02$ and 0.002, where excessive dissipation prevents the growth of the instability. Figure 2 shows volume fraction contours for the modified scheme at the final time step, where the modified dissipation allows the development of a near Mach-independent structure.

An additional issue with low Mach Godunov-type simulations is that the numerical dissipation causes anomalous scaling of the pressure with Mach number [3]. Table I shows the variation of pressure and density differences with respect to Mach. The pressure variations follow the correct Ma^2 scaling; however, the density variations follow that scaling only to $Ma\approx 0.002$, below which there is a departure from the expected behaviour. It is believed that this is due to the problem of 'cancellation' errors. Sesterhenn *et al*. [9] demonstrated that this is a potential issue even at $Ma\approx 0.02$.

4. CONCLUSIONS

This paper has presented a new Roe scheme to solve the multicomponent equations of Wang *et al*. [2] and proposed a modification to this scheme for low Mach flows. This removes the leading order Mach-dependent dissipation and is demonstrated to provide consistent results at Mach numbers as low as 10^{-4}. It also shows correct Ma^2 scaling of pressure fluctuations; however, the density fluctuations deviate from this below $Ma\approx 0.002$. This is believed to be due to cancellation errors.

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