

# POSITIVE SCHEMES AND SHOCK MODELLING FOR COMPRESSIBLE FLOWS

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## SUMMARY

A unified theory of non-oscillatory finite volume schemes for both structured and unstructured meshes is developed in two parts. In the first part, a theory of local extremum diminishing (LED) and essentially local extremum diminishing (ELED) schemes is developed for scalar conservation laws. This leads to symmetric and upstream limited positive (SLIP and USLIP) schemes which can be formulated on either structured or unstructured meshes. The second part examines the application of similar ideas to the treatment of systems of conservation laws. An analysis of discrete shock structure leads to conditions on the numerical flux such that stationary discrete shocks can contain a single interior point. The simplest formulation which meets these conditions is a convective upwind and split pressure (CUSP) scheme, in which the coefficient of the pressure differences is fully determined by the coefficient of convective diffusion. Numerical results are presented which confirm the properties of these schemes.

KEY WORDS: computational aerodynamics; shock capturing; positive schemes

## 1. INTRODUCTION

This paper presents a unified formulation of non-oscillatory discretization schemes for the calculation of compressible flows on both structured and unstructured meshes. Over the past decade the principles underlying the design of non-oscillatory discretization schemes have been quite well established, and numerous variations of artificial diffusion, upwind biasing and flux splitting have been proposed and tested.<sup>1–8</sup> The non-oscillatory properties of the schemes analysed here are secured through the introduction of artificial viscosity which produces an upwind bias. This exactly reproduces an upwind scheme when the minimum sufficient amount of viscosity is used. Higher-order accuracy is obtained by the use of higher-order diffusive terms, with limiters to preserve monotonicity constraints. Schemes which blend low and high-order diffusion,<sup>1</sup> and both symmetric and upstream constructions using anti-diffusive terms controlled by limiters,<sup>9</sup> are readily included within the framework of this paper.

Two main issues arise in the design of non-oscillatory discrete schemes. First there is the issue of how to construct an approximation to a scalar convection or convection–diffusion equation which is non-oscillatory, captures discontinuities with high resolution, and is sufficiently accurate. Second there is the issue of how to construct a numerical flux for a system of equations with waves travelling at different speeds, and sometimes in opposite directions. These two issues can be treated essentially independently, and by combining alternative non-oscillatory formulations with different constructions of the numerical flux one arrives at a matrix of candidate high-

resolution schemes, all of which may have acceptable characteristics. Reference 10 examines the performance of such a matrix of schemes for viscous boundary layers.

Section 2 reviews the conditions for the construction of non-oscillatory schemes for scalar conservation laws. Following a line adhered to in a number of works,<sup>11–14</sup> including several by the present author,<sup>15,8,16</sup> it is suggested that the principle of non-increasing maxima and non-decreasing minima provides a convenient criterion for the design of non-oscillatory schemes. This principle contains the concept of total variation diminishing (TVD) schemes for one-dimensional problems, but can readily be applied to multi-dimensional problems with both structured and unstructured grids. Such local extremum diminishing (LED) schemes can be realized by making sure that the coefficients of the discrete approximation are non-negative. First-order accurate schemes satisfying this principle are easily constructed, but are too diffusive. It is well known that schemes which strictly satisfy the LED principle fall back to first-order accuracy at extrema even when they realize higher-order accuracy elsewhere. This difficulty can be circumvented by relaxing the LED requirement. Therefore, the concept of essentially local extremum diminishing (ELED) schemes is introduced. These are schemes for which, in the limit as the mesh width  $\Delta x \rightarrow 0$ , maxima are non-increasing and minima are non-decreasing.

One approach to the construction of high-resolution schemes which combine monotonicity and higher-order accuracy is to blend low- and high-order diffusive terms as, for example, in the Jameson–Schmidt–Turkel (JST) scheme.<sup>1</sup> Another approach which has been adopted by several authors<sup>12,17–19</sup> is to add limited anti-diffusive terms to a lower-order scheme. This procedure is used here to derive a general family of symmetric limited positive (SLIP) schemes for both structured and unstructured meshes which are LED. Moreover, the limiter can be softened to produce an ELED scheme which preserves second-order accuracy at smooth extrema. It is also shown that the switch in the JST scheme between the low- and high-order diffusive terms can be formulated in such a way that the JST scheme is exactly equivalent to a SLIP scheme. A slight modification of the SLIP—formulation produces a corresponding family of upstream limited positive (USLIP) schemes, which resemble some well-known upwind schemes.<sup>20,7</sup>

Section 3 discusses the treatment of systems of equations with several dependent variables. In order to apply the local extremum diminishing (LED) principle, the flux may be split in a manner which corresponds to the characteristic fields, so that the scheme is designed to limit extrema of the characteristic variables. The Roe flux<sup>4</sup> provides a way to produce schemes that resolve stationary shock waves with a single interior point. The use of a scalar diffusive flux constructed directly from the solution variables leads to simpler schemes which can resolve shock waves with several interior points, and exhibit no overshoots provided that enough diffusion is introduced locally. Because of their low computational costs, scalar diffusive schemes have proved quite suitable for industrial use, and they have been successfully used for aerodynamic analysis in the design of aircraft such as the YF-23.<sup>21</sup> They have the drawback that in order to stabilize the calculation, they tend to introduce more diffusion than is really needed. A formulation of intermediate complexity is to form artificial diffusive terms from a combination of differences of the state and flux vectors. In order to evaluate the shock capturing properties of these various schemes the structure of discrete stationary shocks is analysed, and it is shown that perfect stationary discrete shocks with a single interior point can be obtained both by characteristic decomposition, and by schemes combining differences of the state and flux vectors. These simpler schemes can be formulated by distinguishing the convective and pressure terms, and augmenting each group of terms separately with upwind biasing or diffusive terms. Such convective upwind and split pressure (CUSP) schemes are closely related to the Liou–Steffen flux splitting<sup>22</sup> and also the wave particle splitting proposed by Deshpande and co-workers.<sup>23,24</sup> Scalar diffusion in the right amount, with a coefficient proportional to the minimum eigenvalue of the Jacobian matrix

of the flux vector, produces very sharp discrete shocks, but they are not perfectly free of oscillations.

## 2. NON-OSCILLATORY SCHEMES FOR SCALAR EQUATIONS

### 2.1. Local extremum diminishing (LED) and essentially local extremum diminishing (ELED) schemes

Consider the discretization of a time-dependent conservation law such as

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x} f(v) + \frac{\partial}{\partial y} g(v) = 0 \tag{1}$$

for a scalar-dependent variable  $v$  on an arbitrary (possibly unstructured) mesh. Assuming that the mesh points are numbered in some way, let  $v_j$  be the value at mesh point  $j$ . Suppose that the approximation to (1) is expressed in semi-discrete form as

$$\frac{dv_j}{dt} = \sum_k c_{jk} v_k$$

Then on introducing Taylor series expansions for  $v(x_k - x_j, y_k - y_j)$  it follows that in the absence of a source term

$$\sum_k c_{jk} = 0$$

Thus, there is no loss of generality in writing the scheme as

$$\frac{dv_j}{dt} = \sum_{k \neq j} c_{jk} (v_k - v_j)$$

Suppose that the coefficients are non-negative,

$$c_{jk} \geq 0, \quad k \neq j \tag{2}$$

Then the scheme is stable in the  $L_\infty$  norm, since if  $v_j$  is a maximum,  $v_k - v_j \leq 0$ , so that  $dv_j/dt \leq 0$ , and similarly a minimum cannot decrease. Suppose, moreover, that the stencil of the discrete scheme is compact,

$$c_{jk} = 0 \quad \text{if } j \text{ and } k \text{ are not nearest neighbours} \tag{3}$$

Then if  $v_j$  is a local maximum (over the stencil of the difference scheme)  $v_k - v_j \leq 0$ , with the consequence that  $dv_j/dt \leq 0$ . Thus, a local maximum cannot increase, and similarly a local minimum cannot decrease. Such a scheme will be called local extremum diminishing (LED).

This criterion has been proposed by various authors<sup>11,8,25,13,12</sup> as a convenient basis for the construction of non-oscillatory schemes on both structured and unstructured meshes. It assures positivity, because if  $v$  is everywhere positive, then its global minimum is positive, and this cannot decrease. When specialized to one dimension it also leads to the class of total variation diminishing (TVD) schemes proposed by Harten.<sup>6</sup> The total variation of  $v$  is

$$TV(v) = \int_{-\infty}^{\infty} \left| \frac{dv}{dx} \right| dx$$

that is the sum of the absolute values of the variation over each upward and downward segment. It was observed by Laney and Caughey<sup>13</sup> that each extremum appears in the variation of the

segment on each side of that extremum, with the consequence that

$$TV(v) = 2(\sum \text{maxima} - \sum \text{minima})$$

if the end values are fixed. Thus, if a one-dimensional scheme is LED, it is also TVD. On a triangular mesh, a definition of total variation such as

$$TV(u) = \int \|\nabla u\| dS$$

is not an entirely satisfactory measure of oscillation. This is illustrated in Figure 1, where the total variation of two peaks is found to be less than that of a single ridge. The LED principle, however, continues to be useful for multidimensional problems on both structured and unstructured meshes. Positivity conditions of the type expressed in equations (2) and (3) lead to diagonally dominant schemes, and are the key to the elimination of improper oscillations. The positivity conditions may be realized by the introduction of diffusive terms, or by the use of upwind biasing in the discrete scheme. Unfortunately, they may also lead to severe restrictions on accuracy, unless the coefficients have a complex non-linear dependence on the solution.

Following the pioneering work of Godunov,<sup>26</sup> a variety of dissipative and upwind schemes designed to have good shock capturing properties have been developed during the past two decades.<sup>2-7, 11, 17, 19, 20, 27-31</sup> If the one-dimensional scalar conservation law

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x} f(v) = 0 \tag{4}$$

is represented by a three-point scheme

$$\frac{dv_j}{dt} = c_{j+1/2}^+(v_{j+1} - v_j) + c_{j-1/2}^-(v_{j-1} - v_j)$$

the scheme is LED if

$$c_{j+1/2}^+ \geq 0, \quad c_{j-1/2}^- \geq 0 \tag{5}$$

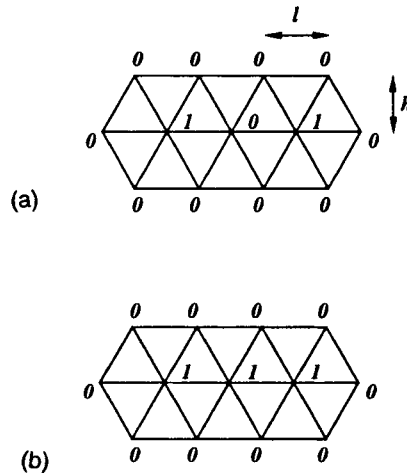


Figure 1. Breakdown of TVD: the one ridge case is less oscillatory than the two peaks case (a) Two Peaks:  $TV = 4 + 2\sqrt{3}$  ( $L_1$ ), 6 ( $L_2$ ), or  $2 + 2\sqrt{3}$  ( $L_\infty$ ). (b) One Ridge:  $TV = 6 + \sqrt{3}$  ( $L_1$ ), 7 ( $L_2$ ), or  $5 + 3\sqrt{3}$  ( $L_\infty$ ).

A conservative semidiscrete approximation to the one-dimensional conservation law can be derived by subdividing the line into cells. Then the evolution of the value  $v_j$  in the  $j$ th cell is given by

$$\Delta x \frac{dv_j}{dt} + h_{j+1/2} - h_{j-1/2} = 0 \quad (6)$$

where  $h_{j+1/2}$  is an estimate of the flux between cells  $j$  and  $j+1$ . The simplest estimate is the arithmetic average  $(f_{j+1} + f_j)/2$ , but this leads to a scheme that does not satisfy the positivity conditions. To correct this, one may add a dissipative term and set

$$h_{j+1/2} = \frac{1}{2}(f_{j+1} + f_j) - \alpha_{j+1/2}(v_{j+1} - v_j)$$

In order to estimate the required value of the coefficient  $\alpha_{j+1/2}$ , let  $a_{j+1/2}$  be a numerical estimate of the wave speed  $\partial f/\partial u$ ,

$$a_{j+1/2} = \begin{cases} (f_{j+1} - f_j)/(v_{j+1} - v_j) & \text{if } v_{j+1} \neq v_j \\ \partial f/\partial v|_{v=v_j} & \text{if } v_{j+1} = v_j \end{cases} \quad (7)$$

Now

$$\begin{aligned} h_{j+1/2} &= f_j + \frac{1}{2}(f_{j+1} - f_j) - \alpha_{j+1/2}(v_{j+1} - v_j) \\ &= f_j - (\alpha_{j+1/2} - \frac{1}{2}a_{j+1/2})(v_{j+1} - v_j) \end{aligned}$$

and similarly

$$h_{j-1/2} = f_j - (\alpha_{j-1/2} + \frac{1}{2}a_{j-1/2})(v_j - v_{j-1})$$

Then

$$h_{j+1/2} - h_{j-1/2} = (\frac{1}{2}a_{j+1/2} - \alpha_{j+1/2})\Delta v_{j+1/2} + (\frac{1}{2}a_{j-1/2} + \alpha_{j-1/2})\Delta v_{j-1/2}$$

where

$$\Delta v_{j+1/2} = v_{j+1} - v_j$$

Thus, the LED condition (5) is satisfied if

$$\alpha_{j+1/2} \geq \frac{1}{2}|a_{j+1/2}| \quad (8)$$

It one takes

$$\alpha_{j+1/2} = \frac{1}{2}|a_{j+1/2}|$$

the diffusive flux becomes

$$d_{j+1/2} = \frac{1}{2}|a_{j+1/2}|\Delta v_{j+1/2}$$

and one obtains the first-order upwind scheme

$$h_{j+1/2} = \begin{cases} f_j & \text{if } a_{j+1/2} > 0 \\ f_{j+1} & \text{if } a_{j+1/2} < 0 \end{cases}$$

This is the least diffusive first-order scheme which satisfies the LED condition. In this sense, upwinding is a natural approach to the construction of non-oscillatory schemes.

Another important requirement of discrete schemes is that they should exclude non-physical solutions which do not satisfy appropriate entropy conditions,<sup>32</sup> which require the convergence of characteristics towards admissible discontinuities. This places more stringent bounds on the

minimum level of numerical viscosity.<sup>33–36</sup> In the case that the numerical flux function is strictly convex, Also<sup>37</sup> has recently proved that it is sufficient that

$$\alpha_{j+1/2} > \max \left\{ \frac{1}{2} |a_{j+1/2}|, \varepsilon \text{sign}(v_{j+1} - v_j) \right\}$$

for  $\varepsilon > 0$ . Thus, the numerical viscosity should be rounded out and not allowed to reach zero at a point where the wave speed  $a(u) = \partial f / \partial u$  approaches zero. This justifies, for example, Harten's entropy fix.

Higher-order schemes can be constructed by introducing higher-order diffusive terms. Unfortunately, these have larger stencils and coefficients of varying sign which are not compatible with the conditions (2) for a LED scheme, and it is known that schemes which satisfy these conditions are at best first-order accurate in the neighbourhood of an extremum. It proves useful in the following development to introduce the concept of essentially local extremum diminishing (ELED) schemes. These are defined to be schemes which satisfy the condition that in the limit as the mesh width  $\Delta x \rightarrow 0$ , local maxima are non-increasing, and local minima are non-decreasing.

## 2.2. High-resolution switched schemes: Jameson–Schmidt–Turkel (JST) scheme

Higher-order non-oscillatory schemes can be derived by introducing anti-diffusive terms in a controlled manner. An early attempt to produce a high-resolution scheme by this approach is the Jameson–Schmidt–Turkel (JST) scheme.<sup>1</sup> Suppose that anti-diffusive terms are introduced by subtracting neighbouring differences to produce a third-order diffusive flux,

$$d_{j+1/2} = \alpha_{j+1/2} \left\{ \Delta v_{j+1/2} - \frac{1}{2} (\Delta v_{j+3/2} + \Delta v_{j-1/2}) \right\} \quad (9)$$

which is an approximation to  $\frac{1}{2} \alpha \Delta x^3 \partial^3 / \partial x^3$ . The positivity condition (2) is violated by this scheme, which proves that it generates substantial oscillations in the vicinity of shock waves. These can be eliminated by switching locally to the first-order scheme. The JST scheme therefore introduces blended diffusion of the form

$$d_{j+1/2} = \varepsilon_{j+1/2}^{(2)} \Delta v_{j+1/2} - \varepsilon_{j+1/2}^{(4)} (\Delta v_{j+3/2} - 2\Delta v_{j+1/2} + \Delta v_{j-1/2}) \quad (10)$$

The idea is to use variable coefficients  $\varepsilon_{j+1/2}^{(2)}$  and  $\varepsilon_{j+1/2}^{(4)}$  which produce a low level of diffusion in regions where the solution is smooth, but prevent oscillations near discontinuities. If  $\varepsilon_{j+1/2}^{(2)}$  is constructed so that it is of order  $\Delta x^2$  where the solution is smooth, while  $\varepsilon_{j+1/2}^{(4)}$  is of order unity, both terms in  $d_{j+1/2}$  will be of order  $\Delta x^3$ .

The JST scheme has proved very effective in practice in numerous calculations of complex steady flows, and conditions under which it could be a total variation diminishing (TVD) scheme have been examined by Swanson and Turkel.<sup>38</sup> An alternative statement of sufficient conditions on the coefficients  $\varepsilon_{j+1/2}^{(2)}$  and  $\varepsilon_{j+1/2}^{(4)}$  for the JST scheme to be LED is as follows.

*Theorem 1 (Positivity of the JST scheme):* Suppose that whenever either  $v_{j+1}$  or  $v_j$  is an extremum the coefficients of the JST scheme satisfy

$$\varepsilon_{j+1/2}^{(2)} \geq \frac{1}{2} |a_{j+1/2}|, \quad \varepsilon_{j+1/2}^{(4)} = 0 \quad (11)$$

Then the JST scheme is local extremum diminishing (LED).

*Proof:* We need only consider the rate of change of  $v$  at extremal points. Suppose that  $v_j$  is an extremum. Then

$$\varepsilon_{j+1/2}^{(4)} = \varepsilon_{j-1/2}^{(4)} = 0$$

and the semi-discrete scheme (6) reduces to

$$\Delta x \frac{dv_j}{dt} = (\varepsilon_{j+1/2}^{(2)} - \frac{1}{2}a_{j+1/2})\Delta v_{j+1/2} - (\varepsilon_{j-1/2}^{(2)} + \frac{1}{2}a_{j-1/2})\Delta v_{j-1/2}$$

and each coefficient has the required sign. □

In order to construct  $\varepsilon_{j-1/2}^{(2)}$  and  $\varepsilon_{j-1/2}^{(4)}$  with the desired properties define

$$R(u, v) = \begin{cases} \left| \frac{u-v}{|u|+|v|} \right|^q & \text{if } u \neq 0 \text{ or } v \neq 0 \\ 0 & \text{if } u = v = 0 \end{cases} \tag{12}$$

where  $q$  is a positive integer. Then  $R(u, v) = 1$  if  $u$  and  $v$  have opposite signs; otherwise  $R(u, v) < 1$ . Now set

$$Q_j = R(\Delta v_{j+1/2}, \Delta v_{j-1/2}), \quad Q_{j+1/2} = \max(Q_j, Q_{j+1})$$

and

$$\varepsilon_{j+1/2}^{(2)} = \alpha_{j+1/2} Q_{j+1/2}, \quad \varepsilon_{j+1/2}^{(4)} = \beta_{j+1/2} (1 - Q_{j+1/2}) \tag{13}$$

where

$$\alpha_{j+1/2} \geq \frac{1}{2}|a_{j+1/2}|, \quad \beta_{j+1/2} \text{ is proportional to } |a_{j+1/2}|$$

At an extremum,  $Q_j = 1$ , since then  $\Delta v_{j+1/2}$  and  $\Delta v_{j-1/2}$  have opposite signs. Elsewhere,  $Q_j \leq 1$  and is of order  $\Delta x$  if the solution is smooth. Thus, the conditions (11) for a LED scheme are satisfied, and if  $q \geq 2$ ,  $\varepsilon_{j+1/2}^{(2)}$  is of order  $\Delta x^2$  in smooth regions not containing an extremum.

### 2.3. Symmetric limited positive (SLIP) scheme

An alternative route to high resolution without oscillation is to introduce flux limiters to guarantee the satisfaction of the positivity condition (2). The use of limiters dates back to the work of Boris and Book.<sup>11</sup> A particularly simple way to introduce limiters, proposed by the author<sup>17</sup> in 1984, is to use flux limited dissipation. In this scheme the third-order diffusion defined by equation (9) is modified by the insertion of limiters which produce an equivalent three-point scheme with positive coefficients. The original scheme<sup>17</sup> can be improved in the following manner so that less restrictive flux limiters are required. Let  $L(u, v)$  be a limited average of  $u$  and  $v$  with the following properties:

- (P1)  $L(u, v) = L(v, u)$ ,
- (P2)  $L(\alpha u, \alpha v) = \alpha L(u, v)$ ,
- (P3)  $L(u, u) = u$ ,
- (P4)  $L(u, v) = 0$  if  $u$  and  $v$  have opposite signs; otherwise,  $L(u, v)$  has the same sign as  $u$  and  $v$ .

Properties (P1)–(P3) are natural properties of an average. Property (P4) is needed for the construction of a LED or TVD scheme.

It is convenient to introduce the notation

$$\phi(r) = L(1, r) = L(r, 1)$$

where according to (P4),  $\phi(r) \geq 0$ . It follows from (P2) on setting  $\alpha = 1/u$  or  $1/v$  that

$$L(u, v) = \phi\left(\frac{v}{u}\right)u = \phi\left(\frac{u}{v}\right)v$$

Also it follows on setting  $v = 1$  and  $u = r$  that

$$\phi(r) = r\phi\left(\frac{1}{r}\right)$$

Thus, if there exists  $r < 0$  for which  $\phi(r) > 0$ , then  $\phi(1/r) < 0$ . The only way to ensure that  $\phi(r) \geq 0$  is to require  $\phi(r) = 0$  for all  $r < 0$ , corresponding to property (P4).

Now one defines the diffusive flux for a scalar conservation law as

$$d_{j+1/2} = \alpha_{j+1/2} \{ \Delta v_{j+1/2} - L(\Delta v_{j+3/2}, \Delta v_{j-1/2}) \} \quad (14)$$

Also define

$$r^+ = \frac{\Delta v_{j+3/2}}{\Delta v_{j-1/2}}, \quad r^- = \frac{\Delta v_{j-3/2}}{\Delta v_{j+1/2}}$$

Then, the scalar scheme (6) reduces to

$$\begin{aligned} \Delta x \frac{dv_j}{dt} &= -\frac{1}{2}a_{j+1/2}\Delta v_{j+1/2} - \frac{1}{2}a_{j-1/2}\Delta v_{j-1/2} + \alpha_{j+1/2}(\Delta v_{j+1/2} - \phi(r^+)\Delta v_{j-1/2}) \\ &\quad - \alpha_{j-1/2}(\Delta v_{j-1/2} - \phi(r^-)\Delta v_{j+1/2}) \\ &= \{ \alpha_{j+1/2} - \frac{1}{2}a_{j+1/2} + \alpha_{j-1/2}\phi(r^-) \} \Delta v_{j+1/2} \\ &\quad - \{ \alpha_{j-1/2} + \frac{1}{2}a_{j-1/2} + \alpha_{j+1/2}\phi(r^+) \} \Delta v_{j-1/2} \end{aligned} \quad (15)$$

Thus, the scheme satisfies the LED condition if  $\alpha_{j+1/2} \geq \frac{1}{2}|a_{j+1/2}|$  for all  $j$ , and  $\phi(r) \geq 0$ , which is assured by property (P4) on  $L$ . At the same time it follows from property (P3) that the first-order diffusive flux is cancelled when  $\Delta v$  is smoothly varying and of constant sign. Schemes constructed by this formulation will be referred to as symmetric limited positive (SLIP) schemes. A variation is to include the coefficient  $\alpha_{j+1/2}$  in the limited average by setting

$$d_{j+1/2} = \alpha_{j+1/2} \Delta v_{j+1/2} - L(\alpha_{j+3/2} \Delta v_{j+3/2}, \alpha_{j-1/2} \Delta v_{j-1/2}) \quad (16)$$

It is easily verified that the argument remains valid. These results may be summarized as follows.

*Theorem 2 (Positivity of the SLIP scheme). Suppose that the discrete conservation law (6) contains a limited diffusive flux as defined by equations (14) or (16). Then the positivity condition (8), together with the properties (P1)–(P4) for limited averages, are sufficient to ensure satisfaction of the LED principle that a local maximum cannot increase and a local minimum cannot decrease.*

The construction benefits from the fact that the terms involving  $\phi(r^-)$  and  $\phi(r^+)$  reinforce the positivity of the coefficients whenever  $\phi$  is positive. Thus, the only major restriction on  $L(u, v)$  is that it must be zero when  $u$  and  $v$  have opposite signs, or that  $\phi(r) = 0$  when  $r < 0$ . If  $\Delta v_{j+3/2}$  and  $\Delta v_{j-1/2}$  have opposite signs then there is an extremum at either  $j$  or  $j+1$ . In the case of an odd–even mode, however, they have the same sign, which is opposite to that of  $\Delta v_{j+1/2}$ , so that they reinforce the damping in the same way that a simple central fourth difference formula would. At the crest of a shock, if the upstream flow is constant then  $\Delta v_{j-1/2} = 0$ , and thus  $\Delta v_{j+3/2}$  is prevented from cancelling any part of  $\Delta v_{j+1/2}$  because it is limited by  $\Delta v_{j-1/2}$ .

A variety of limiters may be defined which meet the requirements of properties (P1)–(P4). Define

$$S(u, v) = \frac{1}{2} \{ \text{sign}(u) + \text{sign}(v) \}$$



so that

$$S(u, v) = \begin{cases} 1 & \text{if } u > 0 \text{ and } v > 0 \\ 0 & \text{if } u \text{ and } v \text{ have opposite sign} \\ -1 & \text{if } u < 0 \text{ and } v < 0 \end{cases}$$

Then two limiters which are appropriate are the following well-known schemes

1. *Minmod*:

$$L(u, v) = S(u, v) \min(|u|, |v|)$$

2. *Van Leer*:

$$L(u, v) = S(u, v) \frac{2|u||v|}{|u| + |v|}$$

In order to produce a family of limiters which contains these as special cases it is convenient to set

$$L(u, v) = \frac{1}{2} D(u, v)(u + v)$$

where  $D(u, v)$  is a factor which should deflate the arithmetic average, and become zero if  $u$  and  $v$  have opposite signs. Take

$$D(u, v) = 1 - R(u, v) = 1 - \left| \frac{u - v}{|u| + |v|} \right|^q \tag{17}$$

where  $R(u, v)$  is the same function that was introduced in the JST scheme, and  $q$  is a positive integer. Then  $D(u, v) = 0$  if  $u$  and  $v$  have opposite signs. Also if  $q = 1$ ,  $L(u, v)$  reduces to minmod, while if  $q = 2$ ,  $L(u, v)$  is equivalent to Van Leer's limiter. By increasing  $q$  one can generate a sequence of limited averages which approach a limit defined by the arithmetic mean truncated to zero when  $u$  and  $v$  have opposite signs. When the ratio  $r = u/v$  is extreme the limiter approaches the asymptotic value

$$\phi(r) = L(1, r) \rightarrow q \text{ as } r \rightarrow \infty$$

When the terms are regrouped, it can be seen that with this limiter the SLIP scheme is exactly equivalent to the JST scheme, with the switch is defined as

$$\begin{aligned} Q_{j+1/2} &= R(\Delta v_{j+3/2}, \Delta v_{j+1/2}) \\ \varepsilon_{j+1/2}^{(2)} &= \alpha_{j+1/2} Q_{j+1/2} \\ \varepsilon_{j+1/2}^{(4)} &= \alpha_{j+1/2} (1 - Q_{j+1/2}) \end{aligned}$$

This formulation thus unifies the JST and SLIP schemes.

2.4. *Essentially local extremum diminishing (ELED) scheme with soft limiter*

The limiters defined by the formula (17) have the disadvantage that they are active at a smooth extrema, reducing the local accuracy of the scheme to first order. In order to prevent this, the SLIP scheme can be relaxed to give an essentially local extremum diminishing (ELED) scheme which is second-order accurate at smooth extrema by the introduction of a threshold in the limited average. Therefore, redefine  $D(u, v)$  as

$$D(u, v) = 1 - \left| \frac{u - v}{\max(|u| + |v|, \varepsilon \Delta x^r)} \right|^q \tag{18}$$

where  $r = \frac{3}{2}$ ,  $q \geq 2$ . This reduces to the previous definition if  $|u| + |v| > \varepsilon \Delta x^r$ . Now

$$d_{j+1/2} = \alpha_{j+1/2} \{ \Delta v_{j+1/2} - \frac{1}{2} D_{j+1/2} (\Delta v_{j+3/2} + \Delta v_{j-1/2}) \}$$

where

$$D_{j+1/2} = D(\Delta v_{j+3/2}, \Delta v_{j-1/2})$$

In any region where the solution is smooth  $\Delta v_{j+3/2} - \Delta v_{j-1/2}$  is of order  $\Delta x^2$ . In fact, if there is a smooth extremum in the neighbourhood of  $v_j$  or  $v_{j+1}$ , a Taylor series expansion indicates that  $\Delta v_{j+3/2}$ ,  $\Delta v_{j+1/2}$  and  $\Delta v_{j-1/2}$  are each individually of order  $\Delta x^2$ , since  $dv/dx = 0$  at the extremum. Then  $D_{j+1/2} = 1 - A$  where  $A$  is of order  $\Delta x^{q/2}$ , and

$$d_{j+1/2} = \alpha_{j+1/2} (\Delta v_{j+1/2} - \frac{1}{2} \Delta v_{j+3/2} - \frac{1}{2} \Delta v_{j-1/2}) + \alpha_{j+1/2} A (\Delta v_{j+3/2} + \Delta v_{j-1/2})$$

where the first term is order  $\Delta x^3$  and the second of order  $\Delta x^{1+q/2}$ . Therefore, taking  $q \geq 2$  is sufficient to ensure at least second-order accuracy at a smooth extremum.

Consider now the possible growth of the extrema. Suppose that  $v_j$  is a maximum, and that  $\Delta v_{j+3/2}$  has the opposite sign to  $\Delta v_{j-1/2}$ , while  $\Delta v_{j-3/2}$  has the opposite sign to  $\Delta v_{j+1/2}$ . Then either  $D_{j+1/2} = 0$  or  $|\Delta v_{j+3/2}| < \varepsilon \Delta x^r$  and  $|\Delta v_{j-1/2}| < \varepsilon \Delta x^r$ . Similarly either  $D_{j-1/2} = 0$ , or  $|\Delta v_{j+1/2}| < \varepsilon \Delta x^r$  and  $|\Delta v_{j-3/2}| < \varepsilon \Delta x^r$ . Now

$$\begin{aligned} \Delta x \frac{dv_j}{dt} &= (\alpha_{j+1/2} + \frac{1}{2} \alpha_{j-1/2} D_{j-1/2} - \frac{1}{2} a_{j+1/2}) \Delta v_{j+1/2} \\ &\quad - (\alpha_{j-1/2} + \frac{1}{2} \alpha_{j+1/2} D_{j+1/2} + \frac{1}{2} a_{j-1/2}) \Delta v_{j-1/2} \\ &\quad - \frac{1}{2} \alpha_{j+1/2} D_{j+1/2} \Delta v_{j+3/2} + \frac{1}{2} \alpha_{j-1/2} D_{j-1/2} \Delta v_{j-3/2} \end{aligned}$$

where  $0 \leq D_{j+1/2} \leq 1$  and  $0 \leq D_{j-1/2} \leq 1$ , and since  $v_j$  is a maximum  $\Delta v_{j+1/2} \leq 0$ ,  $\Delta v_{j-1/2} \geq 0$ . It follows that

$$\Delta x \frac{dv_j}{dt} \leq \frac{1}{2} (\alpha_{j+1/2} + \alpha_{j-1/2}) \varepsilon \Delta x^r$$

If, on the other hand  $\Delta v_{j+3/2}$  has the same sign as  $\Delta v_{j-1/2}$ , it produces a negative contribution to  $dv_j/dt$ . In any case, therefore, if  $v_j$  is a maximum  $dv_j/dt \leq B$ , and similarly if  $v_j$  is a minimum  $dv_j/dt \geq -B$ , where  $B \rightarrow 0$  as  $\Delta x \rightarrow 0$  as long as  $r > 1$ . Thus, the SLIP scheme with the limiter (17) is essentially local extremum diminishing (ELED).

The effect of the 'soft limiter' is not only to improve the accuracy: the introduction of a threshold below which extrema of small amplitude are accepted also usually results in a faster rate of convergence to a steady state, and decreases the likelihood of limit cycles in which the limiter interacts unfavourably with the corrections produced by the updating scheme. In a scheme recently proposed by Venkatakrishnan a threshold is introduced precisely for the purpose.<sup>39</sup>

### 2.5. SLIP schemes on multi-dimensional unstructured meshes

Consider the discretization of the scalar conservation law (1) by a scheme in which  $v$  is represented at the vertices of a triangular mesh, as sketched in Figure 2. In a finite volume approximation, (1) is written in integral form as

$$\frac{d}{dt} \int v \, dS + \oint (f(v) \, dy - g(v) \, dx) = 0$$

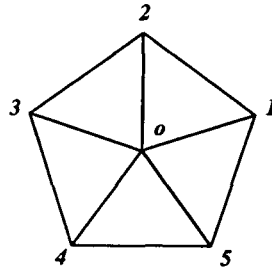


Figure 2. Cell surrounding vertex  $o$

and this is approximated by trapezoidal integration around a polygon consisting of the triangles with a common vertex,  $o$ , say.

Thus, (1) is discretized as

$$S \frac{dv_o}{dt} + \frac{1}{2} \sum_k \{ (f_k + f_{k-1})(y_k - y_{k-1}) - (g_k + g_{k-1})(x_k - x_{k-1}) \} = 0$$

where  $f_k = f(v_k)$ ,  $g_k = g(v_k)$ ,  $S$  is the area of the polygon, and  $k$  ranges over its vertices. This may be rearranged as

$$S \frac{dv_o}{dt} + \sum_k (f_k \Delta y_k - g_k \Delta x_k) = 0$$

where

$$\Delta x_k = \frac{1}{2}(x_{k+1} - x_{k-1}), \quad \Delta y_k = \frac{1}{2}(y_{k+1} - y_{k-1})$$

Following, for example, References 15 and 25, this may now be reduced to a sum of differences over the edges  $ko$  by noting that  $\sum_k \Delta x_k = \sum_k \Delta y_k = 0$ . Consequently  $f_o$  and  $g_o$  may be added to give

$$S \frac{dv_o}{dt} + \sum_k \{ (f_k - f_o) \Delta y_k - (g_k - g_o) \Delta x_k \} = 0 \tag{19}$$

Define the coefficients  $a_{ko}$  as

$$a_{ko} = \begin{cases} \frac{(f_k - f_o) \Delta y_k - (g_k - g_o) \Delta x_k}{\Delta v_{ko}}, & v_k \neq v_o \\ \left( \frac{\partial f}{\partial v} \Delta y_k - \frac{\partial g}{\partial v} \Delta x_k \right) \Big|_{v=v_o}, & v_k = v_o \end{cases}$$

and

$$\Delta v_{ko} = v_k - v_o$$

Then equation (19) reduces to

$$S \frac{dv_o}{dt} + \sum_k a_{ko} \Delta v_{ko} = 0$$

To produce a scheme satisfying the sign condition (2), add a dissipative term on the right-hand side of the form

$$\sum_k \alpha_{ko} \Delta v_{ko} \tag{20}$$

where the coefficients  $\alpha_{ko}$  satisfy the condition

$$\alpha_{ko} \geq |a_{ko}| \tag{21}$$

These simple schemes are far too dissipative. Anti-diffusive terms may be added without violating the positivity condition (2) by the following generalization of the one-dimensional scheme. Considering again the scalar case, let  $\mathbf{l}_{ko}$  be the vector connecting the edge  $ko$  and define the neighbouring differences

$$\Delta^+ v_{ko} = \mathbf{l}_{ko} \cdot \nabla^+ v, \Delta^- v_{ko} = \mathbf{l}_{ko} \cdot \nabla^- v$$

where  $\nabla^\pm v$  are the gradients of  $v$  evaluated in the triangles out of which and into which  $\mathbf{l}_{ko}$  points, as sketched in Figure 3. Arminjon and Dervieux<sup>40</sup> have used a similar definition.

It may now be verified that

$$\Delta^+ v_{ko} = \varepsilon_{pk}(v_p - v_k) + \varepsilon_{qk}(v_q - v_k)$$

and

$$\Delta^- v_{ko} = \varepsilon_{or}(v_o - v_r) + \varepsilon_{os}(v_o - v_s)$$

where the coefficients  $\varepsilon_{pk}$ ,  $\varepsilon_{qk}$ ,  $\varepsilon_{or}$  and  $\varepsilon_{os}$  are all non-negative. Now define the diffusive term for the edge  $ko$  as

$$d_{ko} = \alpha_{ko} \{ \Delta v_{ko} - L(\Delta^+ v_{ko}, \Delta^- v_{ko}) \} \tag{22}$$

where  $L(u, v)$  is a limited average with the properties (P1)–(P4) that were defined in Section 2.3. In considering the sum of the terms at the vertex  $o$  write

$$L(\Delta^+ v_{ko}, \Delta^- v_{ko}) = \phi(r_{ko}^+) \Delta^- v_{ko},$$

where

$$r_{ko}^+ = \frac{\Delta^- k_{ko}}{\Delta^- v_{ko}}$$

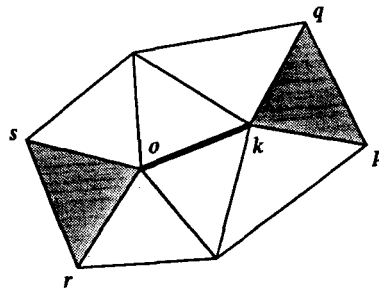


Figure 3. Edge  $ko$  and adjacent triangles

Then, since the coefficients  $\varepsilon_{or}$  and  $\varepsilon_{os}$  are non-negative, and  $\phi(r_{ko}^+)$  is non-negative, the limited antidiffusive term in (22) produces a contribution from every edge which reinforces the positivity condition (2). Similarly, in considering the sum of the terms at  $k$  one writes

$$L(\Delta^+ v_{ko}, \Delta^- v_{ko}) = \phi(r_{ko}^-) \Delta^+ v_{ko}$$

where

$$r_{ko}^- = \frac{\Delta^- v_{ko}}{\Delta^+ v_{ko}}$$

and again the discrete equation receives a contribution with the right sign. One may therefore deduce the following result.

*Theorem 3 (Positivity theorem for unstructured meshes), Suppose that the discrete conservation law (19) is augmented by flux limited dissipation following equations (20) and (22). Then the positivity condition (21), together with the properties (P1)–(P4) for limited averages, are sufficient to ensure the LED property at every interior mesh point.*

Note also that if this construction is applied to any linear function  $v$  then

$$\Delta v_{ko} = \Delta^+ v_{ko} = \Delta^- v_{ko}$$

with the consequence that the contribution of the diffusive terms is exactly zero. In the case of a smoothly varying function  $v$ , suppose that  $\mathbf{l}_{ko} \cdot \nabla v \neq 0$  and the limiter is smooth in the neighbourhood of  $r_{ko}^\pm = 1$ . Then substitution of a Taylor series expansion indicates that the magnitude of the diffusive flux will be of second order. At an extremum the anti-diffusive term is cut off and the diffusive flux is of first order.

### 2.6. Upstream limited positive (USLIP) schemes

By adding the anti-diffusive correction purely from the upstream side one may derive a family of upstream limited positive (USLIP) schemes. Corresponding to the original SLIP scheme defined by equation (14), a USLIP scheme is obtained by setting

$$d_{j+1/2} = \alpha_{j+1/2} \{ \Delta v_{j+1/2} - L(\Delta v_{j+1/2}, \Delta v_{j-1/2}) \}$$

if  $a_{j+1/2} > 0$ , or

$$d_{j+1/2} = \alpha_{j+1/2} \{ \Delta v_{j+1/2} - L(\Delta v_{j+1/2}, \Delta v_{j+3/2}) \}$$

if  $a_{j+1/2} < 0$ . If  $\alpha_{j+1/2} = \frac{1}{2}|a_{j+1/2}|$  one recovers a standard high-resolution upwind scheme in semi-discrete form. Consider the case that  $a_{j+1/2} > 0$  and  $a_{j-1/2} > 0$ . If one sets

$$r^+ = \frac{\Delta v_{j+1/2}}{\Delta v_{j-1/2}}, \quad r^- = \frac{\Delta v_{j-3/2}}{\Delta v_{j-1/2}}$$

the scheme reduces to

$$\Delta x \frac{dv_j}{dt} = -\frac{1}{2} \{ \phi(r^+) a_{j+1/2} + (2 - \phi(r^-)) a_{j-1/2} \} \Delta v_{j-1/2}$$

To assure the correct sign to satisfy the LED criterion the flux limiter must now satisfy the additional constraint that  $\phi(r) \leq 2$ .

The USLIP construction can also be implemented on an unstructured mesh by taking

$$d_{ko} = |a_{ko}| \{ \Delta v_{ko} - L(\Delta v_{ko}, \Delta^- v_{ko}) \}$$

if  $a_{ko} > 0$  and

$$d_{ko} = |a_{ko}| \{ \Delta v_{ko} - L(\Delta v_{ko}, \Delta^+ v_{ko}) \}$$

if  $a_{ko} < 0$ . Let  $\sum^+$  and  $\sum^-$  denote sums over the edges meeting at the vertex  $o$  for which  $a_{ko} > 0$  and  $a_{ko} < 0$ . Define

$$r_{ko}^+ = \frac{\Delta v_{ko}}{\Delta^- v_{ko}}, \quad r_{ko}^- = \frac{\Delta^+ v_{ko}}{\Delta v_{ko}}$$

Then

$$S \frac{dv_o}{dt} = - \sum^+ a_{ko} \phi(r_{ko}^+) \Delta^- v_{ko} - \sum^- a_{ko} (2 - \phi(r_{ko}^-)) \Delta v_{ko}$$

and substituting the formula for  $\Delta^- v_{ko}$  the coefficient of every difference  $\Delta v_{ko}$  is found to be non-negative, with the consequence that the scheme is LED.

### 3. SYSTEMS OF CONSERVATION LAWS

In order to apply similar ideas to a system of equations one may split the flux into components corresponding to the different wave speeds. This concept was first proposed by Steger and Warming.<sup>2</sup> Roe's<sup>4</sup> flux difference splitting is a particularly effective formulation. Consider the one-dimensional case, which may be written in vector notation as

$$\frac{\partial w}{\partial t} + \frac{\partial}{\partial x} f(w) = 0 \quad (23)$$

where  $w$  is the vector of dependent variables, and  $f(w)$  is the flux vector. As in the scalar case, equation (23) may be discretized in finite volume form as

$$\Delta x \frac{dw_j}{dt} + h_{j+1/2} - h_{j-1/2} = 0 \quad (24)$$

where  $h_{j+1/2}$  is the numerical flux through the interface between cells  $j$  and  $j+1$ . This may be expressed as

$$h_{j+1/2} = \frac{1}{2}(f_{j+1} - f_j) - d_{j+1/2} \quad (25)$$

where  $f_j$  denotes  $f(w_j)$ , and  $d_{j+1/2}$  is the diffusive flux.

The wave speeds of the system (23) are the eigenvalues of the Jacobian matrix  $\partial f / \partial w$ . Following Roe,<sup>4</sup> the equations may be locally linearized by introducing a matrix  $A_{j+1/2}$  depending on the states  $w_{j+1}$  and  $w_j$  such that

$$f_{j+1} - f_j = A_{j+1/2}(w_{j+1} - w_j) \quad (26)$$

This corresponds to the definition (7) of  $a_{j+1/2}$  in the scalar case. On introducing the vector

$$v = \begin{pmatrix} \sqrt{\rho} \\ \sqrt{\rho} u \\ \sqrt{\rho} H \end{pmatrix}$$

all quantities in both  $f$  and  $w$  are products of the form  $v^{(j)}v^{(k)}$  which have the property that a finite difference  $\Delta(v^{(j)}v^{(k)})$  between left and right states can be expressed as

$$\Delta(v^{(j)}v^{(k)}) = \bar{v}^{(j)}\Delta v^{(k)} + \bar{v}^{(k)}\Delta v^{(j)}$$

where  $\bar{v}^{(j)}$  is the arithmetic mean  $\frac{1}{2}(v_R^{(j)} + v_L^{(j)})$ . Therefore,

$$\Delta w = B\Delta v, \quad \Delta f = C\Delta v = CB^{-1}\Delta w$$

where  $B$  and  $C$  can be expressed in terms of appropriate mean values of the quantities  $v^{(j)}$ . This is equivalent to evaluating the standard form of the Jacobian matrix  $A = \partial f/\partial w$  using the weighted averages

$$u = \frac{\sqrt{\rho_R}u_R + \sqrt{\rho_L}u_L}{\sqrt{\rho_R} + \sqrt{\rho_L}}, \quad H = \frac{\sqrt{\rho_R}H_R + \sqrt{\rho_L}H_L}{\sqrt{\rho_R} + \sqrt{\rho_L}} \quad (27)$$

and

$$c = \sqrt{(\gamma - 1)(H - u^2/2)} \quad (28)$$

A splitting according to characteristic fields is obtained by decomposing  $A_{j+1/2}$  as

$$A_{j+1/2} = T\Lambda T^{-1}$$

where the columns of  $T$  are the eigenvectors of  $A_{j+1/2}$ , and  $\Lambda$  is a diagonal matrix containing the eigenvalues. Now define a first-order diffusive flux as

$$d_{j+1/2} = \frac{1}{2}|A_{j+1/2}|(w_{j+1} - w_j) \quad (29)$$

where

$$|A_{j+1/2}| = T|\Lambda|T^{-1}$$

and  $|\Lambda|$  is the diagonal matrix containing the absolute values of the eigenvalues. The flux differences can then be expressed as

$$h_{j+1/2} - h_{j-1/2} = (f_{j+1} - f_j)^- + (f_j - f_{j-1})^+$$

where the split flux differences

$$(f_{j+1} - f_j)^\pm = \frac{1}{2}T(\Lambda \pm |\Lambda|)T^{-1}(w_{j+1} - w_j)$$

correspond to the left and right going waves. In order to produce a higher-order SLIP scheme the SLIP construction is applied to the characteristic differences

$$\Delta v_{j+1/2} = T_{j+1/2}^{-1}(w_{j+1} - w_j)$$

Then using superscripts  $k$  to denote the  $k$ th element of  $\Delta v_{j+1/2}$ , define

$$e_{j+1/2}^{(k)} = \frac{1}{2}\hat{\lambda}^k\{\Delta v_{j+1/2}^{(k)} - L(\Delta v_{j+3/2}^{(k)}, \Delta v_{j-1/2}^{(k)})\}$$

where

$$\hat{\lambda}^{(k)} = \begin{cases} |\lambda^{(k)}| & \text{if } |\lambda^{(k)}| > \varepsilon \\ \frac{1}{2}\left(\varepsilon + \frac{|\lambda^{(k)}|^2}{\varepsilon}\right) & \text{if } |\lambda^{(k)}| < \varepsilon \end{cases}$$

Then

$$d_{j+1/2} = T_{j+1/2} e_{j+1/2}$$

$|\lambda^{(k)}|$  is replaced by  $\hat{\lambda}^{(k)}$  to preserve a small amount of diffusion when  $\lambda^{(k)} = 0$ , otherwise, the scheme would support stationary expansion shocks.

### 3.1. Alternative splittings

Characteristic splitting has the advantages that it introduces the minimum amount of diffusion to exclude the growth of local extrema of the characteristic variables, and that with the Roe linearization it allows a discrete shock structure with a single interior point. To reduce the computational complexity one may replace  $|A|$  by  $\alpha$ . If  $\alpha$  is at least equal to the spectral radius  $\max |\lambda(A)|$ , the positivity conditions will still be satisfied. Then the first-order scheme simply has the scalar diffusive flux

$$d_{j+1/2} = \alpha_{j+1/2} \Delta w_{j+1/2}$$

The JST scheme with scalar diffusive flux captures shock waves with about 3 interior points, and it has been widely used for transonic flow calculations because it is both robust and computationally inexpensive.

An intermediate class of schemes can be formulated by defining the first-order diffusive flux as a combination of differences of the state and flux vectors

$$d_{j+1/2} = \alpha_{j+1/2}(w_{j+1} - w_j) + \beta_{j+1/2}(f_{j+1} - f_j)$$

Schemes of this class are fully upwind in supersonic flow if one takes  $\alpha_{j+1/2} = 0$  and  $\beta_{j+1/2} = \text{sign}(M)$  when the absolute value of the Mach number  $M$  exceeds 1. The flux vector  $f$  can be decomposed as

$$f = uw + f_p \tag{30}$$

where

$$f_p = \begin{pmatrix} 0 \\ p \\ up \end{pmatrix} \tag{31}$$

Then

$$f_{j+1} - f_j = \bar{u}(w_{j+1} - w_j) + \bar{w}(u_{j+1} - u_j) + f_{p,j+1} - f_{p,j} \tag{32}$$

where  $\bar{u}$  and  $\bar{w}$  are the arithmetic averages

$$\bar{u} = \frac{1}{2}(u_{j+1} + u_j), \quad \bar{w} = \frac{1}{2}(w_{j+1} + w_j)$$

Thus, these schemes are closely related to schemes which introduce separate splittings of the convective and pressure terms, such as the wave-particle scheme, and the AUSM and CUSP schemes.<sup>22-24,9</sup>

In order to examine the shock capturing properties of these various schemes, consider the general case of a first-order diffusive flux of the form

$$d_{j+1/2} = \frac{1}{2} \alpha_{j+1/2} B_{j+1/2} (w_{j+1} - w_j) \tag{33}$$

where the matrix  $B_{j+1/2}$  determines the properties of the scheme and the scaling factor  $\alpha_{j+1/2}$  is included for convenience. All the previous schemes can be obtained by representing  $B_{j+1/2}$  as



a polynomial in the matrix  $A_{j+1/2}$  defined by equation (26). According to the Cayley–Hamilton theorem, a matrix satisfies its own characteristic equation. Therefore, the third and higher powers of  $A$  can be eliminated, and there is no loss of generality in limiting  $B_{j+1/2}$  to a polynomial of degree 2,

$$B_{j+1/2} = \alpha_0 I + \alpha_1 A_{j+1/2} + \alpha_2 A_{j+1/2}^2 \tag{34}$$

The characteristic upwind scheme for which  $B_{j+1/2} = |A_{j+1/2}|$  is obtained by substituting  $A_{j+1/2} = T\Lambda T^{-1}$ ,  $A_{j+1/2}^2 = T\Lambda^2 T^{-1}$ . Then  $\alpha_0$ ,  $\alpha_1$ , and  $\alpha_2$  are determined from the three equations

$$\alpha_0 + \alpha_1 \lambda_k + \alpha_2 \lambda_k^2 = |\lambda_k|, \quad k = 1, 2, 3$$

The same representation remains valid for three-dimensional flow because  $A_{j+1/2}$  still has only three distinct eigenvalues  $u$ ,  $u + c$ ,  $u - c$ .

### 3.2. Analysis of stationary discrete shocks

The structure of stationary discrete shocks will now be examined under the assumption that the diffusive flux has the form (33). Denote the left and right states by subscripts L and R. The general shock jump condition for a moving shock is

$$f_R - f_L = S(w_R - w_L)$$

where  $S$  is the shock speed. Introducing the Roe linearization between the states  $w_L$  and  $w_R$ , let  $A_{LR}(w_L, w_R)$  be a mean Jacobian matrix with the property that

$$f_R - f_L = A_{LR}(w_R - w_L)$$

Then the shock speed  $S$  is an eigenvalue of  $A_{LR}$ , and  $w_R - w_L$  is the corresponding eigenvector. In the case of a stationary shock  $S = 0$ , the eigenvalues of  $A_{LR}$  are  $u$ ,  $u + c$  and  $u - c$ , and if  $u > 0$  only the eigenvalue  $u - c$  can be zero. It follows that when  $u$  and  $c$  are calculated by equations (27) and (28),  $u = c$  for a stationary shock. Generally, if  $w_A$  is an intermediate state between  $w_L$  and  $w_R$ , and these formulas are used, then for the transition from  $w_L$  to  $w_A$ ,  $u > c$  and for the transition from  $w_A$  to  $w_R$ ,  $u < c$ .

The model of a discrete shock which will be examined is illustrated in Figure 4. Suppose that  $w_L$  and  $w_R$  are left and right states which satisfy the jump conditions for a stationary shock, and that the corresponding fluxes are  $f_L = f(w_L)$  and  $f_R = f(w_R)$ . Since the shock is stationary,  $f_L = f_R$ . The ideal discrete shock has constant states  $w_L$  to the left and  $w_R$  to the right, and a single point with an intermediate value  $w_A$ . The intermediate value is needed to allow the discrete solution to

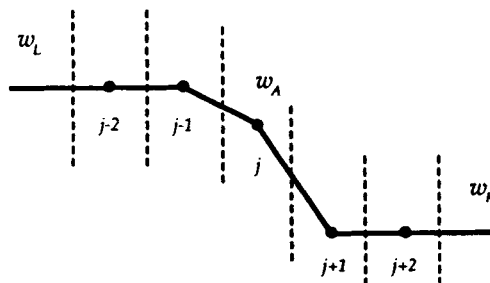


Figure 4. Shock structure for single interior point

correspond to a true solution in which the shock wave does not coincide with an interface between two mesh cells. According to equation (23),

$$\int_0^L w(T) dx = \int_0^L w(0) dx + \int_0^T (f_{RB} - f_{LB}) dt$$

where  $f_{LB}$  and  $f_{RB}$  are the fluxes at the left and right boundaries. Assuming that the boundary conditions are compatible with a steady solution containing a stationary shock, the location  $x_s$  of the shock is fixed by this equation, since

$$\int_0^L w(T) dx = x_s w_L + (L - x_s) w_R$$

Similarly, in the semi-discrete system

$$\sum_j w_j(T) = \sum_j w_j(0) + \int_0^T (f_{RB} - f_{LB}) dt \quad (35)$$

Thus,  $\sum_j w_j(T)$  has a value which is determined by the initial and boundary conditions. In general, it is not possible for this value to be attained by a discrete solution without an intermediate point, because then the sum would be quantized, increasing by  $\Delta_2(w_R - w_L)$  whenever the shock location is shifted one cell to the right.

Three diffusion models of varying complexity which belong to the class defined by equation (34) are examined in the following paragraphs to determine their ability to support the ideal shock structure containing a single interior point. These correspond to one, two or three terms in equation (34).

*3.2.1. Case 1: Scalar Diffusion.* The first model is simple scalar diffusion with  $B_{j+1/2} = I$  and

$$d_{j+1/2} = \frac{1}{2} \alpha_{j+1/2} (w_{j+1} - w_j)$$

Consider the equilibrium in the cell immediately to the right of the shock. Using subscripts AR and RR to denote the values at the cell boundaries, the outgoing flux is

$$h_{RR} = \frac{1}{2} (f_R + f_r) - \frac{1}{2} \alpha_{RR} (w_R - w_r) = f_r$$

while the incoming flux is

$$h_{AR} = \frac{1}{2} (f_R + f_A) - \frac{1}{2} \alpha_{AR} (w_R - w_A)$$

For equilibrium these must be equal. It follows that

$$f_r - f_A + \alpha_{AR} (w_R - w_A) = 0$$

This is the Hugoniot condition for a shock moving to the left with a speed  $\alpha_{AR}$ . Introduce a Roe linearization with a mean Jacobian matrix  $A_{AR}(w_A, w_R)$  such that

$$f_r - f_A = A_{AR} (w_R - w_A)$$

Then  $w_R - w_A$  is an eigenvector of  $A_{AR}$  corresponding to the eigenvalue  $-\alpha_{AR}$ . The eigenvalues of  $A_{AR}$  are  $u$ ,  $u + c$  and  $u - c$ . If we consider flow to the right with  $u > 0$ , and  $u < c$ , a solution with positive numerical diffusion is obtained by taking  $\alpha_{AR} = |u - c|$ . Then the intermediate value  $w_A$  must lie on a Hugoniot curve defined by the right state  $w_R$ .

When the corresponding equilibrium is considered for a cell immediately to the left of a shock wave in a flow moving to the left, it is found that the diffusion coefficient should be  $|u + c|$ . Both cases can be satisfied by taking  $\alpha = \min(|u + c|, |u - c|)$ . In the neighbourhood of a stagnation point the accuracy can be improved by taking  $\alpha$  proportional to  $u$  to prevent the numerical

diffusion becoming undesirably large. This suggests the strategy of using a diffusion coefficient proportional to the smallest eigenvalue, or

$$\alpha_{j+1/2} = \min_k |\lambda_k|$$

where  $\lambda_k$  are the eigenvalues  $u$ ,  $u + c$ , and  $u - c$  of  $A_{j+1/2}$ . To prevent the scheme from admitting stationary expansion shocks which would violate the entropy conditions, the diffusion coefficient may be redefined as

$$\alpha_{j+1/2} = \min_k \hat{\lambda}_k \tag{36}$$

where

$$\hat{\lambda}_k = \begin{cases} |\lambda_k| & \text{if } |\lambda_k| \geq \varepsilon \\ \frac{1}{2} \left( \varepsilon + \frac{|\lambda_k|^2}{\varepsilon} \right) & \text{if } |\lambda_k| < \varepsilon \end{cases} \tag{37}$$

and  $\varepsilon$  is a positive threshold proportional to  $c$ . The usual strategy in schemes using scalar diffusion has been to make the diffusion coefficient proportional to the maximum eigenvalue of the Jacobian matrix  $\partial f / \partial \omega$ , in order to make sure that the numerical viscosity for each characteristic variable is large enough to satisfy the positivity condition. Numerical tests with the alternative strategy of using the smallest eigenvalue confirm that very sharp discrete shocks are obtained, and that the scheme is robust with a viscosity threshold of the type defined by equation (37).

To determine whether scalar diffusion can exactly support an ideal discrete shock it is also necessary to examine the equilibrium in the cell immediately before the shock. In this case the numerical fluxes are

$$h_{LL} = f_L$$

and

$$h_{LA} = \frac{1}{2}(f_A + f_L) - \frac{1}{2}\alpha_{LA}(w_A - w_L)$$

For equilibrium it is necessary that

$$f_A - f_L - \alpha_{LA}(w_A - w_L) = 0$$

which is the Hugoniot condition for a shock moving to the right with a speed  $\alpha_{LA}$ . Introducing the Roe linearization,  $w_A - w_L$  must now be an eigenvector of  $A_{LA}$ . The transition from L to A, however, is less than the full jump for a stationary shock for which it is known that Roe averaging results in  $u = c$ . Thus, it may be expected that  $u > c$ , and the choice  $\alpha_{LA} = u - c = |u - c|$  could still allow the equilibrium condition to be satisfied. Then  $w_A$  lies on a Hugoniot curve defined by the left state  $w_L$ .

The question now arises whether an intermediate state  $w_A$  can be found that simultaneously lies on Hugoniot curves defined by the left and right states  $w_L$  and  $w_R$ , where these two states themselves satisfy the Hugoniot condition for a steady shock. It turns out that this is not possible. Let  $v = 1/\rho$  be the specific volume. Then all possible shocks connecting  $w_L$  and  $w_R$  must satisfy the Hugoniot relation

$$p_R v_R - p_L v_L = \frac{\gamma - 1}{2} (p_R + p_L)(v_L - v_R) \tag{38}$$

This establishes a locus on a  $p$ - $v$  diagram of a family of shocks as the shock speed is varied. The single point shock structure requires  $w_A$  to lie on the Hugoniot curves defined by  $w_L$  and  $w_R$ . The curve defined from  $w_L$  is

$$p_A v_A - p_L v_L = \frac{\gamma - 1}{2} (p_A + p_L)(v_L - v_A) \quad (39)$$

while the curve from  $w_R$  is

$$p_R v_R - p_A v_A = \frac{\gamma - 1}{2} (p_R + p_A)(v_A - v_R) \quad (40)$$

These intersect only when  $w_A = w_R$  or  $w_L$ . To prove this note that (38) can be written as

$$p_R v_R - p_L v_L = \alpha(p_R v_L - p_L v_R) \quad (41)$$

where  $\alpha = (\gamma - 1)/(\gamma + 1)$ . Similarly (39) and (40) yield

$$p_A = p_L \frac{v_L - \alpha v_A}{v_A - \alpha v_L} = p_R \frac{v_R - \alpha v_A}{v_A - \alpha v_R}$$

Thus,  $v_A$  satisfies a quadratic equation. Substituting from equation (41) this can be reduced to

$$(p_R - p_L)(v_A - v_R)(v_A - v_L) = 0$$

If  $p_L \neq p_R$  this has only the solutions  $v_A = v_L$  or  $v_A = v_R$ . Therefore, it is concluded that scalar diffusion cannot support a perfect discrete shock with a single interior point. Calculations of one-dimensional flows reveal an oscillation of very small amplitude upstream of the shock. In multidimensional flows, however, these oscillations are essentially imperceptible.

*3.2.2. Case 2: characteristic upwind scheme.* The second case to be examined is the upwind scheme which results from characteristic decomposition, with  $B_{j+1/2} = |A|_{j+1/2}$ . This case has been studied by Roe,<sup>41</sup> and it is known that the upwind scheme admits ideal shocks. Assuming flow to the right with  $u > 0$ , the fluxes in the cell to the right of the shock are now

$$h_{RR} = f_R$$

and

$$h_{AR} = \frac{1}{2}(f_R + f_A) - \frac{1}{2}|A_{AR}|(w_R - w_A)$$

yielding equilibrium if

$$(A_{AR} - |A_{AR}|)(w_R - w_A) = T(\Lambda - |\Lambda|)T^{-1}(w_R - w_A) = 0$$

With  $u < c$  this is satisfied by the negative eigenvalue  $u - c$ , and since  $w_R - w_A$  is the corresponding eigenvector, the Hugoniot equation

$$f_R - f_A = S(w_R - w_A)$$

is satisfied for the shock speed  $S = u - c$ . Thus,  $w_A$  again lies on a Hugoniot curve. At the entrance to the shock the transition from  $w_L$  to  $w_A$  is less than the full transition from  $w_L$  to  $w_R$  for which  $u = c$ . Thus, a structure is admitted in which  $u > c$  in the transition from L to A, with the consequence that the flux is calculated from the upwind state

$$h_{LA} = \frac{1}{2}(f_A + f_L) - \frac{1}{2}A_{LA}(w_L - w_A) = f_L$$

and equilibrium is maintained.

3.2.3. *Case 3: convective upwind and split pressure (CUSP) scheme.* Characteristic decomposition allows equilibrium to be established through full upwinding of the flux entering the transition layer, while the flux leaving the transition layer satisfies a Hugoniot equation. This can also be accomplished by a less complex scheme. Suppose that the diffusive flux is defined as

$$d_{j+1/2} = \frac{1}{2}\alpha^*c(w_{j+1} - w_j) + \frac{1}{2}\beta(f_{j+1} - f_j)$$

where the factor  $c$  is included so that  $\alpha^*$  is dimensionless. Let  $M$  be the Mach number  $u/c$ . If the flow is supersonic an upwind scheme is obtained by setting

$$\alpha^* = 0, \quad \beta = \text{sign}(M)$$

Introducing the Roe linearization, the Mach number is calculated from  $u$  and  $c$ , and at the entrance to the shock a transition to an intermediate value  $w_A$  is admitted with  $u > c$  and

$$h_{LA} = \frac{1}{2}(f_A + f_L) - \frac{1}{2}(f_A - f_L) = f_L$$

The fluxes leaving and entering the cell immediately to the right of the shock are now

$$f_{RR} = f_R$$

and

$$h_{AR} = \frac{1}{2}(f_R + f_A) - \frac{1}{2}\alpha^*c(w_R - w_A) - \frac{1}{2}\beta(f_R - f_A)$$

These are in equilibrium if

$$f_R - f_A + \frac{\alpha^*c}{1 + \beta}(w_R - w_A) = 0$$

This is the Hugoniot equation for a shock moving to the left with a speed  $\alpha^*c/(1 + \beta)$ . Also, introducing the Roe linearization,

$$\left(A_{RA} + \frac{\alpha^*c}{1 + \beta}I\right)(w_R - w_A) = 0$$

Thus,  $w_R - w_A$  is an eigenvector of  $A_{RA}$  and  $-\alpha^*c/(1 + \beta)$  is the corresponding eigenvalue. Since the eigenvalues are  $u$ ,  $u + c$  and  $u - c$ , the only choice which leads to positive diffusion when  $u > 0$  is  $u - c$ , yielding the relationship

$$\alpha^*c = (1 + \beta)(c - u), \quad 0 < u < c$$

Thus,  $\beta$  is uniquely determined once  $\alpha^*$  is chosen, leading to a one-parameter family of schemes. The choice  $\beta = M$  corresponds to the Harten–Lax–Van Leer (HLL) scheme,<sup>42,43</sup> which is extremely diffusive.

The term  $\beta(f_R - f_A)$  contributes to the diffusion of the convective terms. Suppose that the convective terms are separated by splitting the flux according to equations (30)–(32). Then the total effective coefficient of convective diffusion is

$$\alpha c = \alpha^*c + \beta\bar{u}$$

The choice  $\alpha c = \bar{u}$  leads to low diffusion near a stagnation point, and also leads to a smooth continuation of convective diffusion across the sonic line since  $\alpha^* = 0$  and  $\beta = 1$  when  $|M| > 1$ . The scheme must also be formulated so that the cases of  $u > 0$  and  $u < 0$  are treated symmetrically. Using the notation  $M = u/c$ ,  $\lambda^\pm = u \pm c$ , this leads to the diffusion coefficients

$$\alpha = |M| \tag{42}$$

$$\beta = \begin{cases} +\max\left(0, \frac{u + \lambda^-}{u - \lambda^-}\right) & \text{if } 0 < M < 1 \\ -\max\left(0, \frac{u + \lambda^+}{u - \lambda^+}\right) & \text{if } -1 < M < 0 \\ \text{sign}(M) & \text{if } |M| \geq 1 \end{cases} \quad (43)$$

Near a stagnation point  $\alpha$  may be modified to  $\alpha = \frac{1}{2}(\varepsilon + |M|^2/\varepsilon)$  if  $|M|$  is smaller than a threshold  $\varepsilon$ .

*3.2.4. Criteria for a single point shock.* The analysis of these three cases shows that a discrete shock structure with a single interior point is supported by artificial diffusion that satisfies the two conditions that

1. it produces an upwind flux if the flow is determined to be supersonic through the interface,
2. it satisfies a generalized eigenvalue problem for the exit from the shock of the form

$$(A_{AR} - \alpha_{AR} B_{AR})(w_R - w_A) = 0$$

where  $A_{AR}$  is the linearized Jacobian matrix and  $B_{AR}$  is the matrix defining the diffusion for the interface AR. These two conditions are satisfied by both the characteristic and CUSP schemes. Scalar diffusion does not satisfy the first condition.

### 3.3. CUSP scheme admitting constant total enthalpy in steady flow

In steady flow the stagnation enthalpy  $H$  is constant, corresponding to the fact that the energy and mass conservation equations are consistent when the constant factor  $H$  is removed from the energy equation. Discrete and semi-discrete schemes do not necessarily satisfy this property. In the case of a semi-discrete scheme expressed in viscosity form, equations (24) and (25), a solution with constant  $H$  is admitted if the viscosity for the energy equation reduces to the viscosity for the continuity equation with  $\rho$  replaced by  $\rho H$ . When the standard characteristic decomposition (29) is used, the viscous fluxes for  $\rho$  and  $\rho H$  which result from composition of the fluxes for the characteristic variables do not have this property, and  $H$  is not constant in the discrete solution. In practice there is an excursion of  $H$  in the discrete shock structure which represents a local heat source. In very high-speed flows the corresponding error in the temperature may lead to a wrong prediction of associated effects such as chemical reactions.

The source of the error in the stagnation enthalpy is the discrepancy between the convective terms

$$u \begin{pmatrix} \rho \\ \rho u \\ \rho H \end{pmatrix}$$

in the flux vector, which contain  $\rho H$ , and the state vector which contains  $\rho E$ . This may be remedied by introducing a modified state vector

$$w_h = \begin{pmatrix} \rho \\ \rho u \\ \rho H \end{pmatrix}$$

Then one introduces the linearization

$$f_R - f_L = A_h(w_{h_R} - w_{h_L})$$

Here  $A_h$  may be calculated in the same way as the standard Roe linearization. Introduce the weighted averages defined by equations (27) and (28). Then

$$A_h = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{\gamma + 1}{\gamma} \frac{u^2}{2} & \frac{\gamma + 1}{\gamma} u & \frac{\gamma - 1}{\gamma} \\ -uH & H & u \end{pmatrix}$$

The eigenvalues of  $A_h$  are  $u$ ,  $\lambda^+$  and  $\lambda^-$  where

$$\lambda^\pm = \frac{\gamma + 1}{2\gamma} u \pm \sqrt{\left(\frac{\gamma + 1}{2\gamma} u\right)^2 + \frac{c^2 - u^2}{\gamma}} \tag{44}$$

Note that  $\lambda^+$  and  $\lambda^-$  have the same sign as  $u + c$  and  $u - c$ , and change sign at the sonic line  $u = \pm c$ . The diffusive flux is now expressed as

$$d_{j+1/2} = \frac{1}{2} \alpha^* c \Delta w_h + \frac{1}{2} \beta \Delta f$$

where  $\Delta$  denotes the difference from  $j + 1$  to  $j$ . Now the scheme can be analysed in the same way as before. Again equilibrium at the entrance is established by upwinding, while equilibrium at the exit requires

$$\Delta f + \frac{\alpha^* c}{1 + \beta} \Delta w_h = \left( A_h + \frac{\alpha^* c}{1 + \beta} I \right) \Delta w_h = 0$$

Therefore,  $-\alpha^* c / (1 + \beta)$  must be an eigenvalue of  $A_h$ , and in the case  $u > 0$ , positive diffusion is obtained by taking

$$\alpha^* c = -(1 + \beta) \lambda^-$$

Now the split is redefined as

$$f = u w_h + f_p$$

where

$$f_p = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix}$$

and the diffusive flux can be expressed as

$$d_{j+1/2} = \frac{1}{2} \alpha c \Delta w_h + \beta \bar{w}_h \Delta u + \beta \Delta f_p$$

Then  $\alpha$  and  $\beta$  are defined as before by equations (42) and (43), using the modified eigenvalues  $\lambda^\pm$  defined by equation (44). This splitting corresponds to the Liou–Steffen splitting.<sup>22</sup> The splitting in which the convective terms contain  $\rho E$  corresponds to the wave-particle splitting.<sup>23, 24</sup> The two variations may conveniently be distinguished as the E-CUSP and H-CUSP schemes.

### 3.4. Implementation of limiters for the CUSP scheme

In the case of a scalar conservation law, high-resolution schemes which guarantee the preservation of the positivity or monotonicity of the solution can be constructed by limiting the action of higher order or anti-diffusive terms, which might otherwise cause extrema to grow. Typically these schemes, such as both the symmetric and upstream limited positive (SLIP and USLIP) schemes, compare the slope of the solution at nearby mesh intervals. The characteristic upwind scheme essentially applies the same construction to the characteristic variables, so that the solution is subject to controls on the formulation or growth of extrema of these variables. The fluxes appearing in the CUSP scheme have different slopes approaching from either side of the sonic line, and use of limiters which depends on comparisons of the slopes of these fluxes can lead to a loss of smoothness in the solution at the entrance to a supersonic zone.

An alternative formulation which avoids this difficulty, and which may be used with either the characteristic upwind or the CUSP scheme, is to form the diffusive flux from left and right states at the cell interface. These are interpolated or extrapolated from nearby data, subject to limiters to preserve monotonicity, in a similar manner to the reconstruction of the solution in Van Leer's MUSCL scheme.<sup>27</sup> Let  $w^{(k)}$  denote the  $k$ th element of the state vector  $w$ . Now define left and right states for each dependent variable separately as

$$\begin{aligned}w_L^{(k)} &= w_j^{(k)} + \frac{1}{2}L(\Delta w_{j+3/2}^{(k)}, \Delta w_{j-1/2}^{(k)}) \\w_R^{(k)} &= w_{j+1}^{(k)} - \frac{1}{2}L(\Delta w_{j+3/2}^{(k)}, \Delta w_{j-1/2}^{(k)})\end{aligned}$$

where

$$\Delta w_{j+1/2} = w_{j+1} - w_j$$

and  $L(u, v)$  is a limited average with the properties defined in Section 2.3. Then

$$w_R^{(k)} - w_L^{(k)} = \Delta w_{j+1/2}^{(k)} - L(\Delta w_{j+3/2}^{(k)}, \Delta w_{j-1/2}^{(k)})$$

and in the case of a scalar equation the SLIP scheme is recovered by making the diffusive flux proportional to this difference. To implement the CUSP scheme the pressures  $p_L$  and  $p_R$  for the left and right states are determined from  $w_L$  and  $w_R$ . Then the diffusive flux is calculated by substituting  $w_L$  for  $w_j$  and  $w_R$  for  $w_{j+1}$  to give

$$d_{j+1/2} = \frac{1}{2}\alpha^*c(w_R - w_L) + \frac{1}{2}\beta(f(w_R) - f(w_L))$$

Similarly the characteristic upwind scheme may be implemented by calculating  $A_{j+1/2}$  from  $w_R$  and  $w_L$ .

## 4. TIME STEPPING SCHEMES AND CONVERGENCE ACCELERATION FOR STEADY-STATE CALCULATIONS

### 4.1. Multistage time stepping schemes

The discretization of the spatial derivatives reduces the partial differential equation to a semi-discrete equation which may be written in the form

$$dw/dt + R(w) = 0 \tag{45}$$

where  $w$  is the vector of flow variables at the mesh points, and  $R(w)$  is the vector of the residuals, consisting of the flux balances augmented by the diffusive terms. In the case of a steady-state



calculation the details of the transient solution are immaterial, and the time stepping scheme may be designed solely to maximize the rate of convergence.

If an explicit scheme is used, the permissible time step for stability may be so small that very large number of time steps are needed to reach a steady state. This can be alleviated by using time steps of varying size in different locations, which are adjusted so that they are always close to the local stability limit. If the mesh interval increases with the distance from the body, the time step will also increase, producing an effect comparable to that of an increasing wave speed. Convergence to a steady state can be further accelerated by the use of a multigrid procedure of the type described below.

If one reduces the linear model problem corresponding to (45) to an ordinary differential equation by substituting a Fourier mode  $\hat{w} = e^{ipx_j}$ , the resulting Fourier symbol has an imaginary part proportional to the wave speed, and a negative real part proportional to the diffusion. Thus, the time stepping scheme should have a stability region which contains a substantial interval of the negative real axis, as well as an interval along the imaginary axis. To achieve this it pays to treat the convective and dissipative terms in a distinct fashion. Thus, the residual is split as

$$R(w) = Q(w) + D(w)$$

where  $Q(w)$  is the convective part and  $D(w)$  the dissipative part. Denote the time level  $n\Delta t$  by a superscript  $n$ . Then the multistage time stepping scheme is formulated as

$$\begin{aligned} w^{(n+1,0)} &= w^n \\ &\vdots \\ w^{(n+1,k)} &= w^n - \alpha_k \Delta t (Q^{(k-1)} + D^{(k-1)}) \\ &\vdots \\ w^{n+1} &= w^{(n+1,m)} \end{aligned}$$

where the superscript  $k$  denotes the  $k$ th stage,  $\alpha_m = 1$ , and

$$\begin{aligned} Q_{(0)} &= Q(w^n), \quad D^{(0)} = D(w^n) \\ &\vdots \\ Q^{(k)} &= Q(w^{(n+1,k)}) \\ D^{(k)} &= \beta_k D(w^{(n+1,k)}) + (1 - \beta_k) D^{(k-1)} \end{aligned}$$

The coefficients  $\alpha_k$  are chosen to maximize the stability interval along the imaginary axis, and the coefficients  $\beta_k$  are chosen to increase the stability interval along the negative real axis.

These schemes do not fall within the standard framework of Runge–Kutta schemes, and they have much larger stability regions. Two schemes which have been found to be particularly effective are tabulated below. The first is a four-stage scheme with two evaluations of dissipation. Its coefficients are

$$\begin{aligned} \alpha_1 &= \frac{1}{3}, \quad \beta_1 = 1 \\ \alpha_2 &= \frac{4}{15}, \quad \beta_2 = \frac{1}{2} \\ \alpha_3 &= \frac{5}{9}, \quad \beta_3 = 0 \\ \alpha_4 &= 1, \quad \beta_4 = 0 \end{aligned} \tag{46}$$

The second is a five-stage scheme with three evaluations of dissipation. Its coefficients are

$$\begin{aligned}
 \alpha_1 &= \frac{1}{4}, & \beta_1 &= 1 \\
 \alpha_2 &= \frac{1}{6}, & \beta_2 &= 0 \\
 \alpha_3 &= \frac{3}{8}, & \beta_3 &= 0.56 \\
 \alpha_4 &= \frac{1}{2}, & \beta_4 &= 0 \\
 \alpha_5 &= 1, & \beta &= 0.44
 \end{aligned} \tag{47}$$

#### 4.2. Multigrid

The multigrid scheme is a full approximation scheme defined as follows.<sup>44, 15</sup> Denote the grids by a subscript  $k$ . Start with a time step on the finest grid  $k = 1$ . Transfer the solution from a given grid to a coarser grid by a transfer operator  $P_{k,k-1}$ , so that the initial state on grid  $k$  is

$$w_{(k)}^{(0)} = P_{k,k-1} w_{k-1}$$

Then on grid  $k$  the multistage time stepping scheme is reformulated as

$$w_k^{(q+1)} = w_k^{(0)} - \alpha_n \Delta t (R_k^{(q)} + G_k)$$

where the residual  $R_k^{(q)}$  is evaluated from current and previous values as above, and the forcing function  $G_k$  is defined as the difference between the aggregated residuals transferred from grid  $k-1$  and the residual recalculated on grid  $k$ . Thus,

$$G_k = Q_{k,k-1} R(w_{k-1}) - R(w_k^{(0)})$$

where  $Q_{k,k-1}$  is another transfer operator. On the first stage the forcing term  $G_k$  simply replaces the coarse grid residual by the aggregated fine grid residuals. The accumulated correction on a coarser grid is transferred to the next higher grid by an interpolation operator  $I_{k-1,k}$  so that the solution on grid  $k-1$  is updated by the formula

$$w_{k-1}^{\text{new}} = w_{k-1} + I_{k-1,k} (w_k - w_k^{(0)})$$

The whole set of grids is traversed in a  $W$ -cycle in which time steps are only performed when moving down the cycle.

## 5. NUMERICAL RESULTS

Extensive numerical tests have been performed with a variety of schemes based on the theory presented in this paper. Some of these are reported in references.<sup>9, 45, 46</sup> The schemes have also been evaluated for the treatment of viscous flows.<sup>10, 47</sup> For accurate resolution of the thin boundary layers which appear in flows at high Reynolds numbers, it is important to prevent their contamination by numerical diffusion. The schemes presented here are well suited to this purpose because the artificial diffusion can be made very small as the velocity approaches zero. The SLIP construction also prevents the appearance of overshoots in the velocity profile at high Reynolds numbers. The results presented here will be confined to the CUSP scheme, and are selected to verify the shock capturing properties of the new scheme, in which the coefficients are balanced to support a discrete shock structure with a single interior point.

5.1. One-dimensional shock

In order to verify the discrete structure of stationary shocks, calculations were performed for a one-dimensional problem with initial data containing left and right states compatible with the Rankine Hugoniot conditions. An intermediate state consisting of the arithmetic average of the left and right states was introduced at a single cell in the centre of the domain. With this intermediate state the system is not in equilibrium, and the time-dependent equations were solved

Table I. Shock wave at Mach 20

I	$\rho$	$u$	$H$	$p$	$M$	$s$
1	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
2	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
3	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
4	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
5	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
6	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
7	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
8	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
9	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
10	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
11	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
12	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
13	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
14	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
15	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
16	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
17	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
18	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
19	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
20	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
21	1.0000	23.6643	283.5000	1.0000	20.0000	0.0000
22	4.1924	7.3248	283.4960	307.4467	0.7229	40.3353
23	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
24	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
25	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
26	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
27	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
28	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
29	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
30	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
31	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
32	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
33	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
34	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
35	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
36	5.9259	3.9935	283.4960	466.4889	0.3804	37.6355
37	5.9259	3.9935	283.4960	466.4889	0.3804	37.6354
38	5.9259	3.9935	283.4960	466.4889	0.3804	37.6354
39	5.9259	3.9935	283.4960	466.4889	0.3804	37.6354
40	5.9259	3.9935	283.4961	466.4889	0.3804	37.6355
41	5.9259	3.9935	283.4961	466.4889	0.3804	37.6355
42	5.9259	3.9935	283.4961	466.4889	0.3804	37.6355

to find an equilibrium solution with a stationary shock wave separating the left and right states. Table I shows the result for a shock wave at Mach 20. This calculation used the H-CUSP scheme, which allows a solution with constant stagnation enthalpy. The SLIP construction was used with the limiter defined by equation (18), and  $q = 3$ . The table shows the values of  $\rho$ ,  $u$ ,  $H$ ,  $p$ ,  $M$  and the entropy  $S = \log(p/\rho^\gamma) - \log(p_L/\rho_L^\gamma)$ . A perfect one point shock structure is displayed. The entropy is zero to 4 decimal places upstream of the shock, exhibits a slight excursion at the interior point, and is constant to 4 decimal places downstream of the shock. It may be noted that the mass, momentum and energy of the initial data are not compatible with the final equilibrium state. According to equation (35) the total mass, momentum and energy must remain constant if the outflow flux  $f_R$  remains equal to the inflow flux  $f_L$ . Therefore,  $f_R$  must be allowed to vary

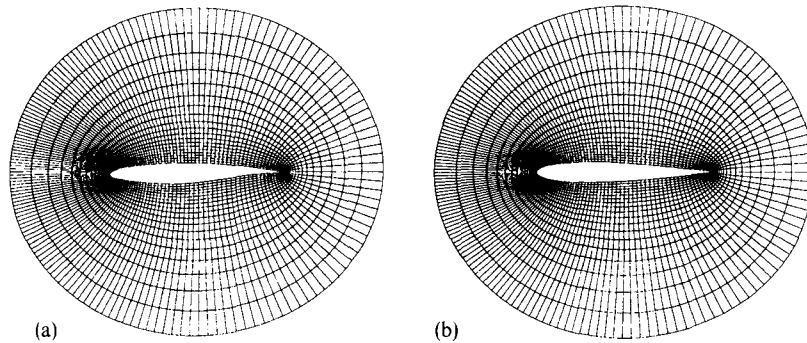


Figure 5. O-topology meshes,  $160 \times 32$  (a) RAE-2822 aerofoil; (b) NACA-0012 aerofoil

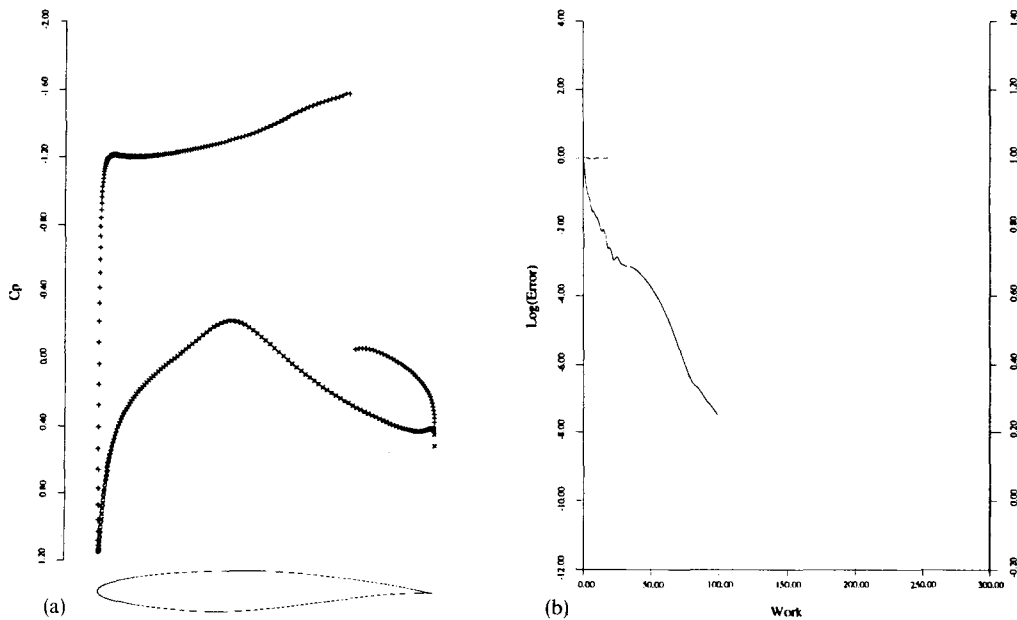


Figure 6. RAE-2822 aerofoil at Mach 0.750 and  $\alpha = 3.0^\circ$  (a)  $C_p$  after 25 cycles.,  $C_l = 1.1312$ ,  $C_d = 0.0469$ ; (b) Convergence, and number of supersonic points

according to an appropriate outflow boundary condition to allow the total mass, momentum and energy to be adjusted to values compatible with equilibrium.

5.2 Aerofoil calculations

The results of transonic flow calculations for two well-known aerofoils, the RAE 2822 and the NACA 0012, are presented in Figures 5–8. The H-CUSP scheme was again used with left and right states defined by the SLIP scheme. The limiter defined by equation (18) was used with  $q = 3$ . The 5 stage time stepping scheme (47) was augmented by the multigrid scheme described in Section 4.2 to accelerate convergence to a steady state. The scheme was simplified by replacing the Roe averages (27) by arithmetic averages, and using  $\lambda^\pm = u \pm c$  in the formula (43) for  $\beta$ . It was also found that the term  $\bar{w}_h \Delta u$  tends to reduce the rate of convergence to a steady state. Therefore, it was attenuated by the factor  $|p_R - p_L| / (|p_R - p_S| + |p_L - p_S|)$  where  $p_S$  is the pressure at sonic speed, and  $p_L$  and  $p_R$  are the pressures to the left and right. When the flow crosses the sonic line  $p_S$  lies between  $p_L$  and  $p_R$ , and this factor becomes unity. Thus, the full scheme is restored at a shock wave. The equations were discretized on meshes with O-topology extending out to a radius of about 100 chords. In each case the calculations were performed on a sequence of successively finer meshes from  $40 \times 8$  to  $320 \times 64$  cells, while the multigrid cycles on each of these meshes descended to a coarsest mesh of  $10 \times 2$  cells. Figure 5 shows the inner parts of the  $160 \times 32$  meshes for the two aerofoils. Figures 6–8 show the final results on  $320 \times 64$  meshes for the RAE 2822 aerofoil at Mach 0.75 and  $3^\circ$  angle of attack, and for the NACA 0012 aerofoil at Mach 0.8 and  $1.25^\circ$  angle of attack, and also at Mach 0.85 and  $1^\circ$  angle of attack. In each case the convergence history is shown for 100 cycles, while the pressure distribution is displayed after

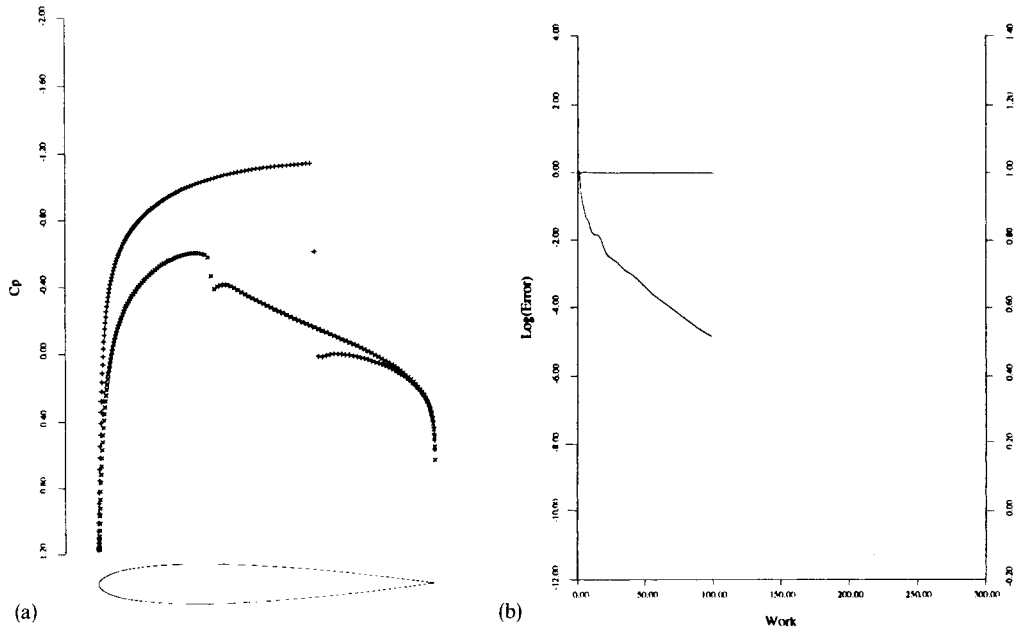


Figure 7. NACA-0012 aerofoil at Mach 0.800 and  $\alpha = 1.25^\circ$  H-CUSP scheme (a)  $C_p$  after 35 Cycles.  $C_l = 0.3654$ ,  $C_d = 0.0232$ ; (b) convergence, and number of supersonic points

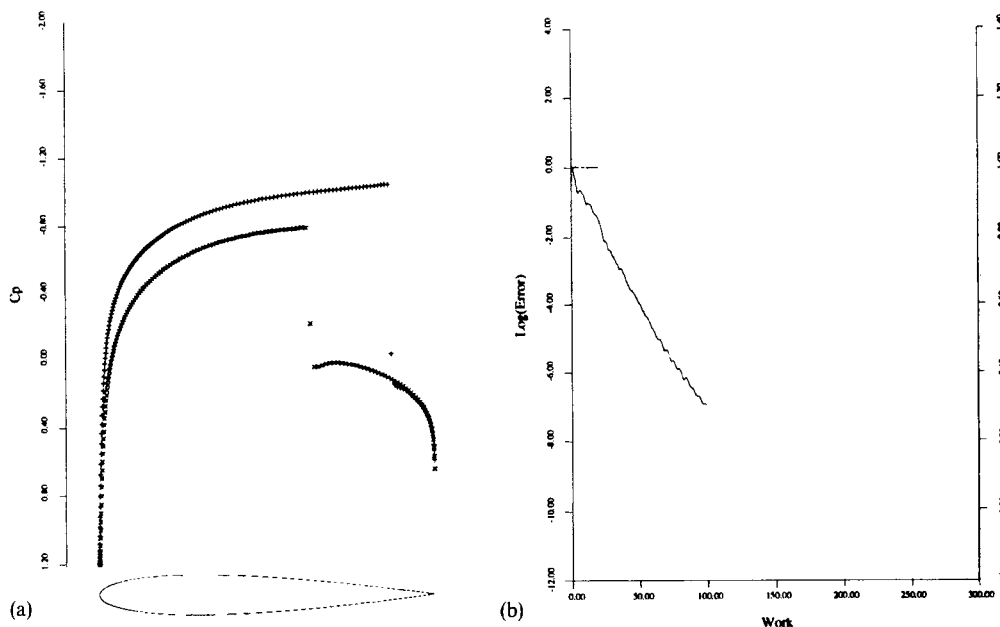


Figure 8. NACA-0012 aerofoil at Mach 0.850 and  $\alpha = 1.0^\circ$  H-CUSP scheme: (a)  $C_p$  after 35 cycles.  $C_l = 0.3861$ ,  $C_d = 0.0582$ ; (b) Convergence, and number of supersonic point

Table II. Drag coefficient on a sequence of meshes

	RAE 2822 Mach 0.50 $\alpha 3^\circ$	NACA 0012 Mach 0.50 $\alpha 3^\circ$	Korn aerofoil Mach 0.75 $\alpha 0^\circ$
$40 \times 8$	0.0062	0.0047	0.0098
$80 \times 16$	0.0013	0.0008	0.0017
$160 \times 32$	0.0000	0.0000	0.0000

a sufficient number of cycles for its convergence. The pressure distribution of the RAE 2822 aerofoil converted in only 25 cycles. Convergence was slower for the NACA 0012 aerofoil. In the case of flow at Mach 0.8 and  $1.25^\circ$  angle of attack, additional cycles were needed to damp out a wave downstream of the weak shock wave on the lower surface.

As a further check on accuracy the drag coefficient should be zero in subsonic flow, or in shock-free transonic flow. Table II shows the computed drag coefficient on a sequence of three meshes for three examples. The first two are subsonic flows over the RAE 2822 and NACA 0012 aerofoils at Mach 0.5 and  $3^\circ$  angle of attack. The third is the flow over the shock free Korn aerofoil at its design point of Mach 0.75 and  $0^\circ$  angle of attack. In all three cases the drag coefficient is calculated to be zero to four digits on a  $160 \times 32$  mesh.

### 5.3. Three-dimensional calculations for a swept wing

As a further test of the performance of the H-CUSP scheme, the flow past the ONERA M6 wing was calculated on a mesh with C-H topology and  $192 \times 32 \times 48 = 294912$  cells. Figure 9

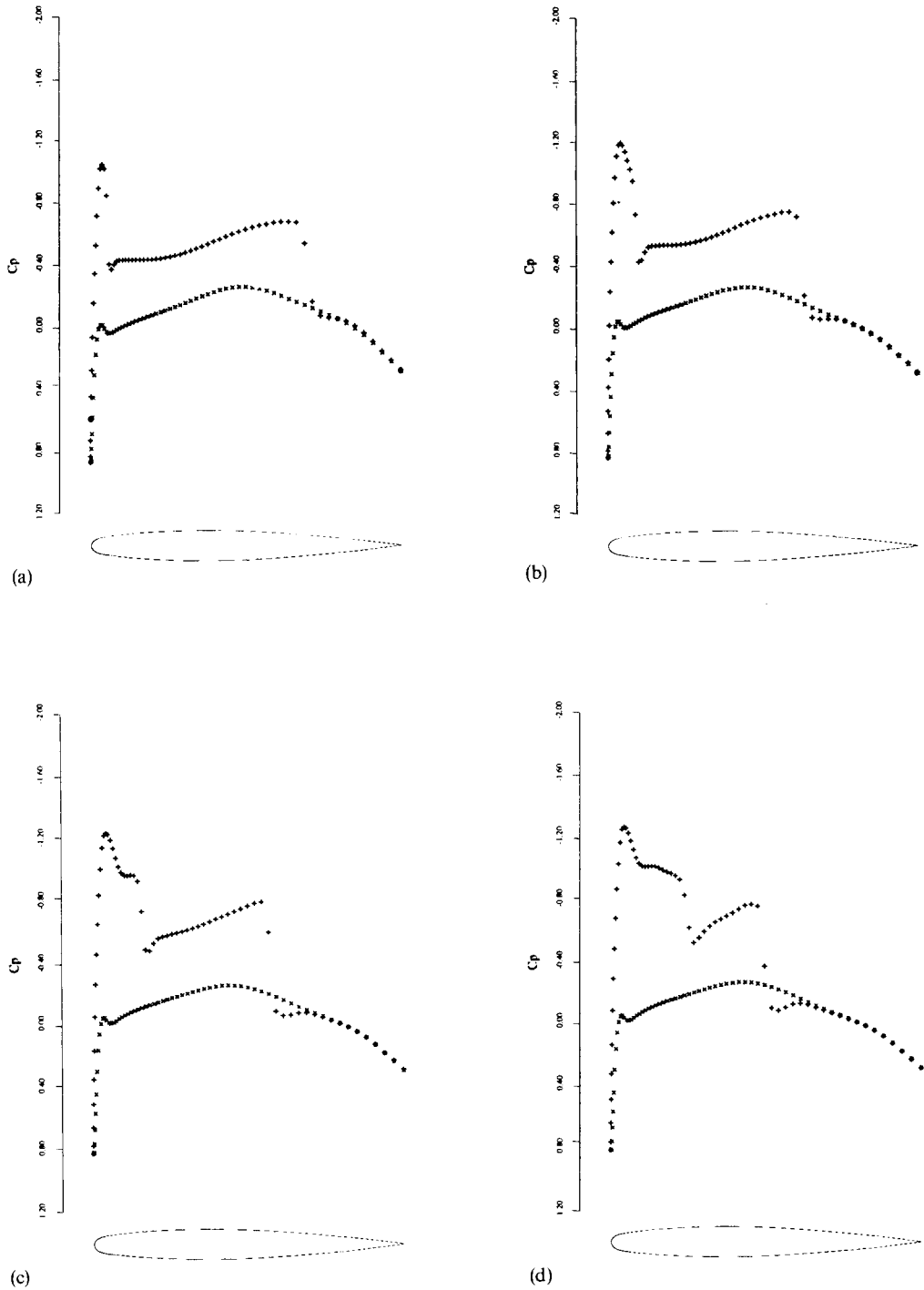


Figure 9. Onera M6 Wing. Mach 0.840, angle of attack 3.06°, 192 × 32 × 48 mesh.  $C_L = 0.3041$ ,  $C_D = 0.0131$ . H-CUSP scheme. (a) 12.50 per cent span.  $C_l = 0.2933$ ,  $C_d = 0.0274$ ; (b) 31.25 per cent span.  $C_l = 0.3139$ ,  $C_d = 0.0159$ ; (c) 50.00 per cent span.  $C_l = 0.3262$ ,  $C_d = 0.0089$ ; (d) 68.75 per cent Span.  $C_l = 0.3195$ ,  $C_d = 0.0026$

shows the result at Mach 0.84 and  $3.06^\circ$  angle of attack. This again verifies the non-oscillatory character of the solution, and the sharp resolution of shock waves. In this case 50 cycles were sufficient for convergence of the pressure distributions.

## 6. CONCLUSION

The concept of local extremum diminishing (LED) schemes provides a convenient framework for the formulation of non-oscillatory shock capturing schemes for compressible flow calculations. In the case of scalar conservation laws the LED property can be secured by corresponding symmetric and upstream limited positive (SLIP and USLIP) schemes. These may be defined in a similar manner for both structured and unstructured meshes. Relaxation of the LED criterion to the less stringent criterion that the scheme should be essentially local extremum diminishing (ELED) allows the use of a 'soft limiter', which preserves second-order accuracy at smooth extrema. The switch in the Jameson–Schmidt–Turler scheme can be formulated so that it reduces to a special case of the SLIP scheme.

The different scalar constructions can be combined with alternate numerical fluxes to provide a matrix of schemes for the gas dynamic equations. The property of supporting stationary discrete shocks with a single interior point is shared by the characteristic and CUSP schemes. The CUSP scheme is computationally inexpensive, and can be formulated to allow solutions with constant stagnation enthalpy in steady flow. It introduces a minimum amount of numerical diffusion as the Mach number approaches zero. It is therefore also appropriate for viscous flow calculations in which it is important not to contaminate the boundary layer.

The theoretical properties of these schemes are verified by numerical calculations of the one-dimensional, two-dimensional and three-dimensional flows.

## ACKNOWLEDGEMENT

This work has benefited from the generous support of ARPA under Grant No. N00014-92-J-1796, AFOSR under Grant No. AFOSR-91-0391, and IBM.

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