High-Order Centered Difference Methods with Sharp Shock Resolution

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Abstract

In this paper we consider high-order centered finite difference approximations of hyperbolic conservation laws. We propose different ways of adding artificial viscosity to obtain sharp shock resolution. For the Riemann problem we give simple explicit formulas for obtaining stationary one- and two-point shocks. This can be done for any order of accuracy. It is shown that the addition of artificial viscosity is equivalent to ensuring the Lax k-shock condition. We also show numerical experiments that verify the theoretical results.

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1 Introduction

Centered finite difference methods, especially high-order ones, are often computationally efficient when the solution of the underlying problem is smooth. For non-smooth solutions, however, these methods produce excessive oscillations, which ultimately will ruin the solutions completely. One way to overcome the spurious phenomena is to introduce numerical viscosity which will smooth the numerical solution. But there are caveats; viscosity must not be used such that unnecessary smoothing occurs. As the computational mesh is refined the viscous effects should decrease while still damping the oscillations. Nessyahu and Tadmor [7] used a Lax-Friedrichs solver to construct non-oscillatory 2nd-order centered difference methods for hyperbolic conservation laws. A similar approach was undertaken by Harten and Lax in [3], where they constructed an approximate Riemann solver from a modified version of Richtmyer's two-step scheme. In this paper we shall develop a general theory on how to achieve sharp shock resolution for high-order finite difference approximations of systems of conservation laws by adding artificial viscosity. We shall thus consider finite difference solutions of the Riemann problem

$$u_t + f_x = 0 u(x,0) = \begin{cases} u_L & x < 0 \\ u_R & x \ge 0, \end{cases}$$
 (1)

where it is assumed that the states u_L , $u_R \in \mathbb{R}^d$ can be connected via a k-shock moving with speed s; $f = f(u) \in \mathbb{R}^d$ is assumed to be differentiable. By means of the coordinate transformation

$$y = x - st$$
$$\tau = t$$

the original Riemann problem (1) is transformed to a stationary problem

$$(f - su)_y = 0 u(y, 0) = \begin{cases} u_L & y < 0 \\ u_R & y \ge 0, \end{cases}$$
 (2)

since $u_{\tau} = 0$ in the (y, τ) -coordinates. It will be assumed that the entropy solution of eq. (2) can be obtained as the pointwise limit (boundedly) of the regularized problem

$$(f - su)_y = L_{\varepsilon}u, \quad \lim_{y \to -\infty} u(y, t) = u_L, \quad \lim_{y \to \infty} u(y, t) = u_R, \tag{3}$$

when $\varepsilon \to 0$; L_{ε} is a linear elliptic operator.

2 Second-Order Difference Methods

When analyzing second-order difference methods we follow the principles set forth in [1, 5]. Hence, eq. (3) is discretized as

$$D_0(f_j - su_j) = \varepsilon h D_+ D_- u_j, \quad \varepsilon > 0,$$
(4)

subject to the boundary conditions

$$\lim_{j \to -\infty} u_j = u_L, \quad \lim_{j \to \infty} u_j = u_R. \tag{5}$$

The right-hand side of eq. (4) corresponds to choosing $L_{\varepsilon} = \varepsilon \partial_y^2$, $\varepsilon \to 0^+$ in eq. (3). The difference operators are defined as

$$D_0 u_j = \frac{1}{2h} (u_{j+1} - u_{j-1}), \quad D_+ u_j = \frac{1}{h} (u_{j+1} - u_j), \quad D_- u_j = \frac{1}{h} (u_j - u_{j-1}),$$

where $h = x_{j+1} - x_j$ is the uniform mesh size. The central difference $D_0(f_j - su_j)$ can be rewritten in conservative form as

$$D_0(f_j - su_j) = D_+ \left(\frac{1}{2} (f_j - su_j + f_{j-1} - su_{j-1}) \right).$$

Thus, eq. (4) can be expressed as

$$D_{+}\left(\frac{1}{2}(f_{j}-su_{j}+f_{j-1}-su_{j-1})-\varepsilon(u_{j}-u_{j-1})\right)=0,$$

which in turn leads to

$$\frac{1}{2}(f_{j+1} - su_{j+1} + f_j - su_j) - \varepsilon(u_{j+1} - u_j) = \frac{1}{2}(f_j - su_j + f_{j-1} - su_{j-1}) - \varepsilon(u_j - u_{j-1})$$

$$= \ldots = f_L - su_L, \tag{6}$$

where the last equality follows from the boundary conditions (5). Consequently,

$$f_{j+1} - f_L - s(u_{j+1} - u_L) - 2\varepsilon u_{j+1} = -(f_j - f_L) + s(u_j - u_L) - 2\varepsilon u_j$$

Let

$$\begin{array}{lcl} F(u) & = & f(u) - f_L - s(u - u_L) - 2\varepsilon u \\ G(u) & = & f_L - f(u) + s(u - u_L) - 2\varepsilon u \,. \end{array}$$

The difference approximation (4), (5) can then be written as

$$F(u_{j+1}) = G(u_j). (7)$$

Letting $j \to \infty$ yields

$$F(u_R) = G(u_R),$$

i. e.,

$$f_R - f_L = s(u_R - u_L). (8)$$

This is the familiar Rankine-Hugoniot condition, which is fulfilled since u_L and u_R are the states on either side of the stationary k-shock problem (2). We can thus define F(u) and G(u) as

$$F(u) = f(u) - f_P - s(u - u_P) - 2\varepsilon u$$

$$G(u) = f_P - f(u) + s(u - u_P) - 2\varepsilon u,$$
(9)

where $u_P = u_L$ or $u_P = u_R$. The second choice corresponds to letting $j \to \infty$ in eq. (6). The Rankine-Hugoniot condition would then follow by taking the limit $j \to -\infty$ in eq. (7).

2.1 Nonlinear Analysis of One- and Two-Point Shocks

Given that there exists a solution, eq. (7) can be interpreted in the following way: The two states u_L and u_R can be connected to each other via a stationary viscous profile $\{u_j\}_{-\infty}^{\infty}$ where u_j satisfies the nonlinear recursion formula (7). The question then arises naturally whether it is possible to connect two given states u_L and u_R by a viscous profile consisting of a *finite* number of intermediate states u_{M_j} , $j = 1, \ldots, p$. We begin by proving a negative result.

Proposition 2.1 There are no states $u_L \neq u_R$ such that u_L and u_R can be coupled by the viscous regularization (7) without any intermediate state, i. e., there are no zero-point shocks.

Proof: Suppose that the two states u_L and u_R can be directly coupled by eq. (7), i. e.,

$$F(u_R) = G(u_L).$$

From definition (9) it follows immediately that

$$f_R - f_P - s(u_R - u_P) - 2\varepsilon u_R = f_P - f_L + s(u_L - u_P) - 2\varepsilon u_L$$

But the Rankine-Hugoniot condition (8) implies that

$$2\varepsilon u_R = 2\varepsilon u_L .$$

Since $\varepsilon > 0$ it follows that $u_R = u_L$, which proves the proposition.

Proposition 2.2 Two states u_L , $u_R \in \mathbb{R}^d$ can be connected via a viscous profile (7) using one intermediate state $u_M \in \mathbb{R}^d$ (one-point shock). Furthermore, if the states u_L and u_R are close, the Lax k-shock condition is equivalent to having $\varepsilon > 0$ in eq. (4).

Proof: A single intermediate state u_M must according to eq. (7) satisfy

$$G(u_L) = F(u_M)$$

$$G(u_M) = F(u_R).$$
(10)

The definition of F and G and the Rankine-Hugoniot condition (8) together imply that

$$-2\varepsilon u_L = f_M - f_L - s(u_M - u_L) - 2\varepsilon u_M$$

$$-2\varepsilon u_R = f_L - f_M + s(u_M - u_L) - 2\varepsilon u_M$$
 (11)

Adding these two equation yields

$$u_M = \frac{1}{2}(u_L + u_R). (12)$$

We have thus found the intermediate state u_M . The scalar viscosity ε and the shock speed s remain to be determined. Using the well-known Roe-linearization one can rewrite eq. (11) as

$$(A(u_L, u_M) - sI)(u_L - u_M) = 2\varepsilon(u_L - u_M)$$

$$(A(u_M, u_R) - sI)(u_M - u_R) = -2\varepsilon(u_M - u_R),$$
(13)

where the Roe-matrices $A(u_L, u_M)$ and $A(u_M, u_R)$ are defined by

$$A(u_L, u_M) = \int_0^1 f'(\theta u_L + (1 - \theta)u_M)d\theta$$

$$A(u_M, u_R) = \int_0^1 f'(\theta u_M + (1 - \theta)u_R)d\theta.$$

But eq. (13) has a solution if and only if

$$2\varepsilon = \mu_k(u_L, u_M) - s$$
, $2\varepsilon = -\mu_k(u_M, u_R) + s$,

i. e.,

$$\varepsilon = \frac{1}{4} (\mu_k(u_L, u_M) - \mu_k(u_M, u_R))$$

$$s = \frac{1}{2} (\mu_k(u_L, u_M) + \mu_k(u_M, u_R)).$$
(14)

Here $\mu_k(u_L, u_M)$ and $\mu_k(u_M, u_R)$ denote eigenvalues of $A(u_L, u_M)$ and $A(u_M, u_R)$, respectively. From the definitions of the Roe-matrices it follows immediately that

$$A(u_L, u_L) = f'(u_L), \quad A(u_R, u_R) = f'(u_R).$$

Denote by $\lambda_k(u)$ the eigenvalues of f'(u). Hence, Taylor expansion yields

$$\mu_k(u_L, u_M) = \lambda_k(u_L) + \mathcal{O}(|u_M - u_L|) = \lambda_k(u_L) + \mathcal{O}(|u_R - u_L|),$$

where the second equality follows from eq. (12). Similarly,

$$\mu_k(u_M, u_R) = \lambda_k(u_R) + \mathcal{O}(|u_R - u_L|)$$
.

The Lax k-shock condition requires that

$$\lambda_k(u_L) > s > \lambda_k(u_R)$$

hold for exactly one characteristic family k, $1 \le k \le d$. Thus, for weak shocks the Lax k-shock condition holds iff

$$\mu_k(u_L, u_M) > s > \mu_k(u_M, u_R),$$

which in turn implies that $\varepsilon > 0$, i. e., eq. (4) satisfies an entropy inequality. Conversely, suppose that $\varepsilon > 0$. Then

$$\mu_k(u_L, u_M) > \mu_k(u_M, u_R).$$

Hence,

$$\mu_k(u_L, u_M) > \frac{1}{2}(\mu_k(u_L, u_M) + \mu_k(u_M, u_R)) > \mu_k(u_M, u_R).$$

Recalling eq. (14) we see that

$$\mu_k(u_L, u_M) > s > \mu_k(u_M, u_R).$$

Thus, for weak shocks our solutions obey the Lax k-shock condition.

Finally, we need to verify that s defined by eq. (14) is compatible with the Rankine-Hugoniot condition (8). We have

$$f_L - f_R = A(u_L, u_M)(u_L - u_M) + A(u_M, u_R)(u_M - u_R).$$

For a one-point shock, however, $u_L - u_M$, $u_M - u_R$ are eigenvectors of $A(u_L, u_M)$ and $A(u_M, u_R)$ (cf. eq. (13)), respectively, whence

$$f_L - f_R = \mu_k(u_L, u_M)(u_L - u_M) + \mu_k(u_M, u_R)(u_M - u_R)$$

Using eq. (12) yields

$$f_L - f_R = \frac{1}{2} (\mu_k(u_L, u_M) + \mu_k(u_M, u_R))(u_L - u_R).$$

Thus, the Rankine-Hugoniot condition (8) is satisfied with

$$s = \frac{1}{2}(\mu_k(u_L, u_M) + \mu_k(u_M, u_R)).$$

This concludes the proof.

Remark: The proof of the previous proposition shows that one should choose ε according to eq. (14). In the actual implementation, however, it would be advantageous to use

$$\varepsilon = \frac{1}{4} |\mu_k(u_L, u_M) - \mu_k(u_M, u_R)|,$$

since the argument of the modulus function would be positive for a true k-shock. If, on the other hand, the argument should happen to be negative due to round-off errors, for instance, then the modulus function will prevent the formation of an entropy violating shock.

In the scalar case ε and s can be expressed directly in terms of f(u) since

$$\mu_k(u_L, u_M) = A(u_L, u_M) = \frac{f_L - f_M}{u_L - u_M} = \frac{2(f_L - f_M)}{u_L - u_R}$$

$$\mu_k(u_M, u_R) = A(u_M, u_R) = \frac{f_M - f_R}{u_M - u_R} = \frac{2(f_M - f_R)}{u_L - u_R}$$

Using these expressions in eq. (14) yields

$$\varepsilon = \frac{f_L - 2f_M + f_R}{2(u_L - u_R)}$$

$$s = \frac{f_L - f_R}{u_L - u_R}$$
(15)

The next proposition shows that the smallness assumption of proposition 2.2 is not needed for strictly convex scalar functions f(u).

Proposition 2.3 Let f(u) be a twice differentiable, strictly convex scalar function, and let ε be given by eq. (15). Then

$$\varepsilon > 0 \iff f'(u_L) > f'(u_R)$$
.

Remark: The latter condition is the well-known entropy condition for scalar conservation laws [6].

Proof: Taylor expansion yields

$$f_R = f(u_R - u_M + u_M) = f(u_M) + f'(u_M)(u_R - u_M) + \frac{1}{2}f''(w)(u_R - u_M)^2$$

$$f_L = f(u_L - u_M + u_M) = f(u_M) + f'(u_M)(u_L - u_M) + \frac{1}{2}f''(v)(u_L - u_M)^2$$

for some v and w. Using eq. (12) then gives

$$\varepsilon = \frac{f_L - 2f_M + f_R}{2(u_L - u_R)} = \frac{1}{16} \left(f''(v) + f''(w) \right) \left(u_L - u_R \right).$$

But f'' > 0 because of strict convexity. Hence,

$$\varepsilon > 0 \Longleftrightarrow u_L > u_R \Longleftrightarrow f'(u_L) > f'(u_R)$$
.

The second equivalence follows since f'(u) is a strictly increasing function of u (because of strict convexity).

Example: For Burgers' equation the flux is given by

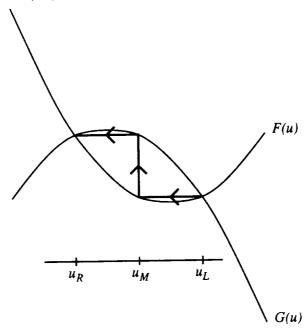
$$f(u) = \frac{1}{2}u^2.$$

From eq. (15) it then follows that

$$\varepsilon = \frac{1}{8}(u_L - u_R)$$

$$s = \frac{1}{2}(u_L + u_R).$$
(16)

In case of a convex scalar function f(u) the one-point shock condition (10) can be depicted as (recall that $F(u_L) = G(u_L)$, $F(u_R) = G(u_R)$)



Thus far we have shown how to obtain a one-point shock. It is not necessary to confine ourselves to one-point shocks, which the following discussion will show. Suppose that we want to connect u_L and u_R by a viscous profile using two intermediate states u_{M_1} and u_{M_2} . This amounts to requiring

$$G(u_L) = F(u_{M_1})$$

$$G(u_{M_1}) = F(u_{M_2})$$

$$G(u_{M_2}) = F(u_R).$$
(17)

Adding these three equations yields

$$u_{M_2} - u_{M_1} = \frac{1}{2}(u_R - u_L). \tag{18}$$

As before we rewrite the first and third equations of (17) as

which can be solved iff

$$2\varepsilon = \mu_k(u_L, u_{M_1}) - s > 0 \qquad u_{M_1} - u_L = \alpha_1 r_k(u_L, u_{M_1}) \\ -2\varepsilon = \mu_k(u_{M_2}, u_R) - s < 0 \qquad u_{M_2} - u_R = \alpha_2 r_k(u_{M_2}, u_R),$$

where $r_k(u_L, u_{M_1})$, $r_k(u_{M_2}, u_R)$ denote the kth eigenvectors of $A(u_L, u_{M_1})$, $A(u_{M_2}, u_R)$. The inequalities are immediate consequences of the k-shock condition. The first set of

equations yields

$$\varepsilon = \frac{1}{4} (\mu_k(u_L, u_{M_1}) - \mu_k(u_{M_2}, u_R))$$

$$s = \frac{1}{2} (\mu_k(u_L, u_{M_1}) + \mu_k(u_{M_2}, u_R)).$$
(19)

In particular, if u_{M_1} and u_{M_2} are known, so are ε and s. The intermediate states are determined by eq. (18), by

$$u_{M_1} - u_L = \alpha_1 r_k(u_L, u_{M_1}) u_{M_2} - u_R = \alpha_2 r_k(u_{M_2}, u_R),$$
 (20)

and by the Rankine-Hugoniot conditions (8). As opposed to the case of a one-point shock, the explicit eigenvector structure of $A(u_L, u_{M_1})$ and $A(u_{M_2}, u_R)$ must be known in order to compute the intermediate states.

Example: In the scalar case eq. (20) becomes redundant $(r_k = 1)$. We are thus left with

$$u_{M_2} - u_{M_1} = (u_R - u_L)/2$$

$$f_R - f_L = s(u_R - u_L)$$

$$s = (\mu(u_L, u_{M_1}) + \mu(u_{M_2}, u_R))/2,$$

i. e.,

$$\frac{f_L - f_{M_1}}{u_L - u_{M_1}} + \frac{f_{M_2} - f_R}{u_{M_2} - u_R} = \frac{2(f_L - f_R)}{u_L - u_R}$$
(21)

$$u_{M_2} - u_{M_1} = (u_R - u_L)/2$$
.

For Burgers' equation one gets the linear system

$$u_{M_1} + u_{M_2} = u_L + u_R$$

 $u_{M_1} - u_{M_2} = (u_L - u_R)/2$,

which yields

$$u_{M_1} = (3u_L + u_R)/4$$

 $u_{M_2} = (u_L + 3u_R)/4$.

Consequently,

$$\mu(u_L, u_{M_1}) = \frac{1}{8}(7u_L + u_R), \quad \mu(u_{M_2}, u_R) = \frac{1}{8}(u_L + 7u_R),$$

which implies

$$\varepsilon = \frac{3}{16}(u_L - u_R)$$

$$s = \frac{1}{2}(u_L + u_R).$$
(22)

2.2 Linear Perturbation Analysis

In general we cannot expect the methods based on nonlinear analysis to be insensitive to perturbations. A different approach could be based upon linearization of eq. (7) [1, 5]:

$$(f'(u_P) - sI)u_{j+1} - 2\varepsilon u_{j+1} = -(f'(u_P) - sI)u_j - 2\varepsilon u_j.$$

This equation can be diagonalized when f'(u) corresponds to a hyperbolic operator. The diagonalization is formally obtained by letting $f'(u_P) \to \lambda_P$, $I \to 1$. We thus obtain

$$(\lambda_P - s - 2\varepsilon)u_{j+1} = (-\lambda_P + s - 2\varepsilon)u_j$$
.

Suppose that $u_P = u_R$. This corresponds to linearizing around the state to the *right* of the shock. We can thus express u_{j+1} as a function of u_j :

$$u_{j+1} = \frac{-\lambda_R + s - 2\varepsilon}{\lambda_R - s - 2\varepsilon} u_j,$$

where u_j is assumed to be to the right of the shock. Note that one could not reverse the recursion above, since one would ultimately cross the discontinuity, across which the linearization has no meaning. The linearization implies that u_j is viewed as a perturbation around the constant state u_R . No matter what the value of u_j is, we can make the perturbation disappear in the next step by setting

$$s - 2\varepsilon = \lambda_R. \tag{23}$$

Similarly, linearizing around the left state u_L gives

$$u_j = \frac{\lambda_L - s - 2\varepsilon}{-\lambda_L + s - 2\varepsilon} u_{j+1},$$

where it now is assumed that u_{j+1} is to the left of the shock. Again, requiring

$$s + 2\varepsilon = \lambda_L \tag{24}$$

implies that perturbations are annihilated in one step. Combining eqs. (23), (24) yields

$$\varepsilon = \frac{1}{4}(\lambda_L - \lambda_R)$$

$$s = \frac{1}{2}(\lambda_L + \lambda_R).$$
(25)

The above expression for s states that s is the arithmetic average of the characteristic speeds on either side of the shock. This is the correct value modulo second order terms [6]. In particular, one should expect the corresponding numerical scheme to work well for weak shocks. Note that the analysis thus far – linear as well as nonlinear – has been based on eq. (7), which was obtained from eq. (4) by factoring out the operator D_+ .

Example: For Burgers' equation we have $\lambda_P = u_P$, whence

$$\varepsilon = \frac{1}{4}(u_L - u_R)$$

$$s = \frac{1}{2}(u_L + u_R).$$
(26)

In the above example the linear approach resulted in twice as much viscosity as the one-point-shock. Note that the shock speed s is unchanged. This is, however, a coincidence. The values of ε and s are determined by two criteria, namely that perturbations to the left and to the right of the shock are annihilated in one step. In general, these requirements are incompatible with correct shock speed (cf. eqs. (14), (25)), i. e., the Rankine-Hugoniot condition. Of course, if we confine ourselves to eliminating the oscillations on only one side of the shock, then we can use the correct shock speed.

The transformation of eq. (1) to the time independent problem (2) was done to enable the theoretical analysis. In practice, one often computes in the fixed coordinate frame of eq. (1), which requires no a priori knowledge about s; correct shock speed will follow from the conservation form of (1). However, one can use the values for ε obtained from the theoretical analysis and still obtain good results, cf. subsequent sections. Furthermore, in practical implementations it would be desirable to implement the viscosity locally around the shock. This can be done by introducing a switch so as to turn off the viscosity in the smooth regime. One way to do this would be to replace the right-hand side of eq. (4) by

$$\varepsilon D_+ r_{j-1/2} D_- u_j \,,$$

where $r_j = 1$ close to the shock, $r_j = 0$ otherwise; $r_{j-1/2}$ is the interpolation of r_j at the cell interface $x_{j-1/2}$; u_L and u_R would be replaced by some interpolated value of u to the left and the right of the shock, respectively.

3 High-Order Difference Methods

We shall now use the results from the previous sections for 2nd-order methods to construct artificial viscosity for high-order methods. The standard explicit centered approximation of $\partial/\partial x$ of order 2r has the form

$$Q_{2\tau} = R_{2\tau} D_0 \,, \tag{27}$$

$$R_{2\tau} = \sum_{\nu=0}^{\tau-1} (-1)^{\nu} \alpha_{\nu} (h^2 D_+ D_-)^{\nu} , \qquad (28)$$

where the coefficients α_{ν} are defined by

$$\alpha_0 = 1,
\alpha_{\nu} = \frac{\nu}{4\nu + 2} \alpha_{\nu - 1}, \quad \nu = 1, 2, \dots, r - 1.$$
(29)

We can also use compact implicit difference approximations of Padé type. Some of these operators can be written in the form (27), but with a different operator $R_{2\tau}$. For example, the compact 4th-order approximation is (27) with

$$R_4 = R_4^{(i)} = \left(I + \frac{h^2}{6}D_+D_-\right)^{-1}. \tag{30}$$

We will always assume that the implicit operators have the form $R^{(i)} = P^{-1}$, where P is a nonsingular explicit operator of finite bandwidth.

3.1 Factorization of High-Order Dissipation

The idea to use to construct the viscosity, is to use high-order dissipation $h \in D$, where D can be factored as $D = R_{2r}D_+D_-$. The approximation for the transformed equation (2) is

$$R_{2r}D_0(f - su)_j = h\varepsilon R_{2r}D_+D_-u_j,$$
 (31)

where ε is a parameter. The boundary conditions are as before

$$\lim_{j \to -\infty} u_j = u_L, \quad \lim_{j \to \infty} u_j = u_R. \tag{32}$$

By (31) we see that it is natural to consider the operator $R_{2\tau}$ in the space \mathcal{M} of grid functions $\{v_j\}$ with

$$\lim_{j \to \pm \infty} v_j = 0. \tag{33}$$

By definition, the inverse of the implicit operators exist. For the explicit operators we have

Lemma 3.1 The explicit operator R_{2r} in (28) is non-singular in the space \mathcal{M} .

Proof: Consider the equation

$$R_{2r}v_j = 0, \ j = 0, \pm 1, \dots$$
 (34)

for real v_j , and let the scalar product and norm be defined by

$$(v, w) = \sum_{j=-\infty}^{\infty} v_j w_j h, \quad ||v||^2 = (v, v).$$

Summation by parts yields (using (34) and (33))

$$0 = (v, R_{2r}v) = ||v||^2 + \sum_{\nu=1}^{r-1} (-1)^{\nu} \alpha_{\nu}(v, (h^2D_+D_-)^{\nu}v)$$

$$= ||v||^2 + \sum_{\nu=1}^{r-1} \alpha_{\nu} ||(hD_{-})^{\nu}v||^2.$$

Note that the boundary terms disappear because of (33). Since all α_{ν} are positive, it follows that v=0, which proves the lemma.

Since R_{2r} is non-singular, the equation (31) holds if and only if

$$D_0(f - su)_i = h\varepsilon D_+ D_- u_i \tag{35}$$

holds. But this is the three-point scheme that we have analyzed in section 2. Therefore, the high-order methods with artificial viscosity, as in (31), produce exactly the same solution as the three-point scheme does. To take advantage of the high-order approximation property, we must obviously implement the viscosity locally around the discontinuity. We use the same switch function r_j as for the three-point scheme. We summarize the results in

Proposition 3.1 The propositions in section 2 concerning zero- and one-point shocks for 2nd-order methods apply to high-order methods of the form (31) as well. For one-point shocks ε should be chosen according to eq. (14). Here R_{2r} is defined either by the explicit formula (28), or by an implicit operator as described above.

In section 2 we also determined the viscosity coefficient ε based on linear analysis. The linearized equation for the high-order methods is

$$R_{2r}D_0(f'(u_P) - sI)u_j = h\varepsilon R_{2r}D_+D_-u_j.$$
 (36)

The arguments in section 2 can be applied to this equation, and the optimal choice of ε for the three-point scheme is optimal in the same sense for the high-order method.

For explicit operators $R_{2\tau}$, the effect of the artificial viscosity can be interpreted in the following way. Upon diagonalization, the general solution of (36) is given by

$$u_j = \sum_{\nu=1}^{2r} \sigma_\nu \kappa_\nu^j \,, \tag{37}$$

where $\kappa_{\nu} = \kappa_{\nu}(\varepsilon)$ are the roots of the characteristic equation; σ_{ν} are arbitrary scalar coefficients. For $\varepsilon = 0$ there are two roots

$$\kappa_1 = 1$$
, $\kappa_2 = -1$.

There are also r-1 roots $\{\kappa_{\nu}\}_{3}^{r+1}$ with $|\kappa_{\nu}(0)| < 1$, and r-1 roots $\{\kappa_{\nu}\}_{r+2}^{2r}$ with $|\kappa_{\nu}(0)| > 1$, see [9]. All roots except $\kappa_{1} = 1$ give rise to parasitic solutions, and $\kappa_{2} = -1$ is the one that causes the trouble. The remaining roots also induce errors, but they are less severe. If $|\kappa_{\nu}| > 1$, then its presence near the shock is not felt, since the solution is bounded as $j \to \infty$. The analogous arguments hold for the solution to the left of the shock. The special choice (25) of ε for the three-point scheme gives $\kappa_{2} = 0$. The factored form (36) implies that the coefficients σ_{ν} , $\nu = 3, 4, \ldots, 2r$ vanish. This follows since

 R_{2r} is nonsingular on the space \mathcal{M} , which means that eq. (36) is equivalent to eq. (4). Consequently, the general solution (37) is identical to that of a three-point scheme. But that is possible iff the coefficients $\sigma_{\nu} = 0$, $\nu = 3, 4, \ldots, 2r$; the roots κ_{ν} , $\nu = 3, 4, \ldots, 2r$ are non-zero, but they do not influence the solution. Hence, the solution of the linear equation has the form

 $u_j = \sigma_1 \,, \tag{38}$

where σ_1 is determined by the condition at $x_j = \infty$, i. e., $\sigma_1 = u_R$.

3.2 High-Order Dissipation Based on Perturbation Analysis

We shall now consider a different form of artificial viscosity for the explicit approximation. For the nonlinear equation we use

$$R_{2\tau}D_0(f - su)_j = \sum_{\nu=1}^{\tau} h^{2\nu-1} \varepsilon_{\nu} (D_+ D_-)^{\nu} u_j.$$
 (39)

This choice of viscosity corresponds to having $L_{\varepsilon} = \sum_{\nu=1}^{r} \varepsilon_{\nu} \partial_{y}^{2\nu}$, $\varepsilon_{\nu} \to 0$ in eq. (3). There are r viscosity coefficients to determine, but the width of the total difference operator is not increased by the viscosity terms. The linearized equation is

$$R_{2r}D_0(f'(u_P) - sI)u_j = \sum_{\nu=1}^r h^{2\nu-1} \varepsilon_{\nu} (D_+ D_-)^{\nu} u_j.$$
 (40)

The general form of the solution is still given by (37). Instead of forcing the coefficients $\sigma_3, \sigma_4, \ldots, \sigma_{2r}$ to vanish, we now choose ε_{ν} such that

$$\kappa_2 = \kappa_3 = \ldots = \kappa_{r+1} = 0,$$

where, as before,

$$|\kappa_{\nu}| < 1 \;, \; \nu = 3, 4, \; \dots \; r+1$$

when no viscosity is present. This procedure can also be viewed as reducing the linear approximation to an r+1 point scheme near the shock. As above we implement the approximation with a switch r_j . After a re-normalization $(j \to j - N)$ the solution of the linearized equation can be expressed as

$$u_j = \sigma_1 + \sum_{\nu=r+2}^{2r} \sigma_{\nu} \kappa_{\nu}^{j-N} , \quad |\kappa_{\nu}| > 1.$$
 (41)

The parasitic part of the solution represented by the sum does not cause any harm. Even if the computation is carried out over a finite domain, such that $j \leq N$, where N is fixed, the coefficients σ_{ν} are bounded since the solution is bounded at j = N. Therefore, $\sigma_{\nu} \kappa_{\nu}^{j-N}$ is small near the shock where j << N. We do not expect any difficulties, even if the shock passes through the boundary, since our methods are either strictly or strongly stable, see [8, 2].

In the analysis we have assumed that all roots κ_{ν} are simple. Should there be multiple roots, $\{\kappa_{\nu}\}_{3}^{2r}$ can always be partitioned into one group with exactly r-1 members inside the unit circle and another group with r-1 members outside the unit circle. Hence, our principle still applies. All the κ_{ν} inside the unit circle vanish by our choice of ε_{ν} .

We illustrate our principle by considering a 4th-order approximation Q_4 . After diagonalization eq. (40) becomes

$$(12\varepsilon_{2} + \lambda_{P} - s)u_{j+2} + (12\varepsilon_{1} - 48\varepsilon_{2} - 8(\lambda_{P} - s))u_{j+1} - (24\varepsilon_{1} - 72\varepsilon_{2})u_{j}$$

$$+ (12\varepsilon_{1} - 48\varepsilon_{2} + 8(\lambda_{P} - s))u_{j-1} + (12\varepsilon_{2} - \lambda_{P} + s)u_{j-2} = 0$$

$$(42)$$

Suppose that we have linearized eq. (39) to the right of the shock, i. e., $u_P = u_R$. We now want to eliminate the characteristic roots $\kappa_2 = -1$ and κ_3 , $|\kappa_3| < 1$. Being to the right of the shock this corresponds to setting the coefficients in front of u_{j-1} and u_{j-2} to zero $(j = k, k+1, \ldots)$. Hence,

$$\varepsilon_1 = -\frac{1}{3}(\lambda_R - s)$$

$$\varepsilon_2 = \frac{1}{12}(\lambda_R - s).$$
(43)

On the other hand, linearizing eq. (39) to the left of the shock corresponds to setting $u_P = u_L$ in eq. (42). This time we set the coefficients in front of u_{j+1} and u_{j+2} to zero (j = -k, -k - 1, ...), thus resulting in

$$\varepsilon_1 = \frac{1}{3}(\lambda_L - s)$$

$$\varepsilon_2 = -\frac{1}{12}(\lambda_L - s).$$
(44)

One realizes immediately from eqs. (43) and (44) that $\varepsilon_1 > 0$, $\varepsilon_2 < 0$ is equivalent to the k-shock condition $\lambda_L > s > \lambda_R$. The viscosity coefficients will be uniquely determined iff (cf. remarks at the end of section 2.2)

$$s = \frac{1}{2}(\lambda_L + \lambda_R).$$

Thus,

$$\varepsilon_{1} = \frac{1}{6} (\lambda_{L} - \lambda_{R})$$

$$\varepsilon_{2} = -\frac{1}{24} (\lambda_{L} - \lambda_{R})$$

$$s = \frac{1}{2} (\lambda_{L} + \lambda_{R}).$$
(45)

Using these values in eq. (42) yields

$$(\lambda_{L} - \lambda_{P})u_{j+2} - 8(\lambda_{L} - \lambda_{P})u_{j+1} + 7(\lambda_{L} - \lambda_{R})u_{j}$$

$$-8(\lambda_{P} - \lambda_{R})u_{j-1} + (\lambda_{P} - \lambda_{R})u_{j-2} = 0.$$
(46)

Hence, to the right of the shock we obtain $(\lambda_L \neq \lambda_R)$

$$u_{j+2} - 8u_{j+1} + 7u_j = 0, \quad j = k, k+1, \dots$$

Similarly,

$$7u_{j} - 8u_{j-1} + u_{j-2} = 0$$
, $j = -k, -k-1, \dots$

to the left of the shock. Using the substitution $j \to -j$ in the latter equation and defining $v_j = u_{-j}$, the two recursive expressions above will coalesce into

$$u_{j+2} - 8u_{j+1} + 7u_j = 0, \quad j = k, k+1, \dots$$

whose characteristic roots are given by

$$\kappa_1 = 1, \quad \kappa_4 = 7.$$

Summing up, choosing s, ε_1 , and ε_2 according to eq. (45) in eq. (40) (for r=2) yields the following characteristic roots

$$\kappa_1 = 1, \quad \kappa_2 = 0, \quad \kappa_3 = 0, \quad \kappa_4 = 7.$$

Thus, the parasitic modes corresponding to κ_2 and κ_3 have been eliminated.

Example: For Burgers' equation we have $\lambda_P = u_P$, whence

$$\varepsilon_1 = \frac{1}{6}(u_L - u_R)$$

$$\varepsilon_2 = -\frac{1}{24}(u_L - u_R)$$

$$s = \frac{1}{2}(u_L + u_R).$$

$$(47)$$

Numerical results for this approximation will be presented in section 5.

3.3 Averaging Operators

Yet a different kind of viscosity, based on simple 2nd-order averaging, was used in [2]. We consider the approximation of the problem in its original time dependent form

$$\frac{du_j}{dt} + Q_{2r}f_j = 0. (48)$$

Let

$$\tilde{u}_j^{n+1} = P(\tilde{u}_j^n)$$

be a time discretization of Runge-Kutta type of the high-order semi-discrete difference scheme (48). Then the algorithm is

$$\tilde{u}_{j}^{n+1} = P(u_{j}^{n})
u_{j}^{n+1} = (\tilde{u}_{j-1}^{n+1} + 2\tilde{u}_{j}^{n+1} + \tilde{u}_{j+1}^{n+1})/4$$
(49)

Linearize around a constant state away from the shock as was done earlier. Let

$$\frac{dv_j}{dt} = S_{2\tau}v_j \,, \quad S_{2\tau} = -Q_{2\tau}f'(u_P)$$

be the linearized difference approximation in space without any viscosity. Then the Runge-Kutta method is

$$\tilde{v}_j^{n+1} = P(kS_{2r})v_j^n \,, \tag{50}$$

where

$$P(z) = 1 + \sum_{\nu=1}^{m} \beta_{\nu} z^{\nu}$$

is a polynomial (third degree in our experiments), and k is the time step. The averaging procedure can be written as

$$v_j^{n+1} = (I + \frac{h^2}{4}D_+D_-)\tilde{v}_j^{n+1}.$$

Hence, one complete step with the filtered Runge-Kutta method for the linearized equation is

$$v_j^{n+1} = P(kS_{2\tau})v_j^n + \frac{h^2}{4}D_+D_-P(kS_{2\tau})v_j^n.$$

For explicit approximations Q_{2r} the artificial viscosity contains difference operators of all orders between 2 and m(2r-1)+2, i. e., odd order terms will appear. For implicit approximations Q_{2r} all grid points are involved when the filter is applied at any given point. With steady state solutions one obtains

$$\frac{1}{k}(I - P(kS_{2\tau}))v_j = -\frac{h}{4\lambda}D_+D_-P(kS_{2\tau})v_j,$$

where $\lambda = k/h$. Hence, the viscosity coefficients depend on the Courant number. In the last section it is demonstrated that the averaging technique (implemented with a switch function) is also very efficient for non-stationary shocks.

4 Linear Discontinuities

Consider the linear problem

$$u_t + \mu u_x = 0$$

$$u(x,0) = \varphi(x)$$
(51)

where φ is the (possibly discontinuous) periodic initial data; $\mu \in \Re$. The equation above can be discretized as

$$u_j^{n+1} = u_j^n - k\mu D_0 u_j^n + \varepsilon kh D_+ D_- u_j^n,$$
 (52)

or

$$u_j^{n+1} = \lambda \left(\varepsilon + \frac{\mu}{2} \right) u_{j-1}^n + \left(1 - 2\varepsilon \lambda \right) u_j^n + \lambda \left(\varepsilon - \frac{\mu}{2} \right) u_{j+1}^n,$$

where $\lambda = k/h$. It is well-known that by choosing

$$\varepsilon = \frac{|\mu|}{2} \tag{53}$$

one gets an upwind scheme. Furthermore, requiring

$$\lambda = \frac{1}{2\varepsilon} = \frac{1}{|\mu|} \Longleftrightarrow k = \frac{h}{|\mu|} \tag{54}$$

results in the method of characteristics, i. e.,

$$u_i^{n+1} = u_{i-1}^n \text{ if } \mu > 0, \quad u_j^{n+1} = u_{j+1}^n \text{ if } \mu < 0.$$

Now suppose that ∂_x is approximated using the high-order operator $Q_{2r} = R_{2r}D_0$. We can then use the idea from section 3.1 to obtain the following implicit scheme

$$R_{2r}u_i^{n+1} = R_{2r}u_i^n - k\mu Q_{2r}u_i^n + \varepsilon kh R_{2r}D_+D_-u_j^n.$$
 (55)

Assuming that there exists a periodic solution of eq. (55), it follows that R_{2r}^{-1} exists. In the class of periodic solutions eq. (55) is thus equivalent to eq. (52). Hence, the conclusions above also pertain to eq. (55).

In regions where the flow is smooth it should not be necessary to resort to the method of characteristics in order to compute solutions of high accuracy. Consider an explicit 4th-order method for convenience. The viscosity term is then modified according to

$$\varepsilon h R_4 D_+ r_{j-1/2} D_- , \quad R_4 = I - \frac{h^2}{6} D_+ r_{j-1/2} D_- ,$$
 (56)

where $r_{j-1/2} = 0.5(r_{j-1} + r_j)$ is the interpolant of a switch function r_j ; $Q_4 = (I - (h^2/6)D_+D_-)D_0$. We have used a switch proposed by Jameson [4]

$$r_j = \left(\frac{|\Delta_+ u_j - \Delta_- u_j|}{|\Delta_+ u_j| + |\Delta_- u_j|}\right)^p . \tag{57}$$

Note that $r_j = 1$ if $\Delta_- u_j$ and $\Delta_+ u_j$ do not have the same sign. In particular, $r_j = 1$ where there are high-frequent oscillations. Choosing $p = \infty$ ensures that $r_j = 0$ at the grid points where the flow is smooth. Thus, in smooth regions we have $R_4 = I$. Assuming that the spurious phenomena are localized to a compact set it follows that R_4 is non-singular. Eq. (51) is now discretized by

$$R_{4}u_{j}^{(1)} = R_{4}u_{j}^{n} - \lambda L_{4}u_{j}^{n}$$

$$R_{4}u_{j}^{(2)} = \alpha_{j}R_{4}u_{j}^{n} + \beta_{j}R_{4}u_{j}^{(1)} - \gamma_{j}\lambda L_{4}u_{j}^{(1)}$$

$$R_{4}u_{i}^{n+1} = \delta_{j}R_{4}u_{i}^{n} + \eta_{j}R_{4}u_{i}^{(2)} - \zeta_{j}\lambda L_{4}u_{j}^{(2)},$$
(58)

where R_4 is defined by (56); the spatial operator L_4 is given by

$$L_4 = hQ_4 - \varepsilon h^2 R_4 D_+ r_{i-1/2} D_- \tag{59}$$

and the integration parameters are given by

$$\alpha_{j} = 3/4
\beta_{j} = 1/4
\gamma_{j} = 1/4
\delta_{j} = 1/3
\delta_{j} = 0,
\gamma_{j} = 0
\delta_{j} = 0
\delta_{j} = 0
\delta_{j} = 0
if $r_{j} = 1$. (60)
 $\eta_{j} = 2/3$ $\eta_{j} = 1$
 $\zeta_{j} = 2/3$ $\zeta_{j} = 0$$$

Now, in smooth regions where $r_j = 0$ the discretization (58) reduces to $(R_4 = I, L_4 = Q_4)$

$$u_j^{(1)} = u_j^n - \lambda Q_4 u_j^n$$

$$u_j^{(2)} = \frac{3}{4} u_j^n + \frac{1}{4} u_j^{(1)} - \frac{\lambda}{4} Q_4 u_j^{(1)}$$

$$u_j^{n+1} = \frac{1}{3} u_j^n + \frac{2}{3} u_j^{(2)} - \frac{2\lambda}{3} Q_4 u_j^{(2)},$$

which is a 3rd-order TVD Runge-Kutta method. Note in particular that the value of ε is irrelevant whenever $r_j = 0$. When $r_j = 1$, on the other hand, we recover

$$R_4 u_i^{n+1} = R_4 u_i^n - k \mu Q_4 u_i^n + \varepsilon k h R_4 D_+ D_- u_i^n.$$

Should $r_j = 1$ for all j this is nothing but the Euler forward method (where we have assumed periodicity) that reduces to an upwind method for $\varepsilon = |\mu|/2$ and to the method of characteristics for $\lambda = 1/|\mu|$. If $r_j = 1$ locally, we expect (58) to behave roughly like an upwind scheme in that region.

Returning to the original formulation (58) we observe that since R_4 is non-singular, eq. (58) can be written in explicit form

$$u_{j}^{(1)} = u_{j}^{n} - \lambda v_{j}^{n}
 u_{j}^{(2)} = \alpha_{j} u_{j}^{n} + \beta_{j} u_{j}^{(1)} - \gamma_{j} \lambda v_{j}^{(1)}
 u_{j}^{n+1} = \delta_{j} u_{j}^{n} + \eta_{j} u_{j}^{(2)} - \zeta_{j} \lambda v^{(2)},$$
(61)

where v^n , $v^{(1)}$ and $v^{(2)}$ are the solutions of the tridiagonal systems

$$R_4 v_j^n = L_4 u_j^n$$
, $R_4 v_j^{(i)} = L_4 u_j^{(i)}$, $i = 1, 2$.

The tridiagonal structure of R_4 is given by

$$R_4 v_j = \frac{1}{6} \left(-r_{j-1/2} v_{j-1} + (6 + r_{j+1/2} + r_{j-1/2}) u_j - r_{j+1/2} u_{j+1} \right) .$$

In the next section we will present numerical results obtained from (61).

5 Numerical Results

We begin by studying the factorized artificial viscosity described in section 3.1. We have used the explicit and implicit 4th-order schemes (31), obtained by setting

$$R_{2\tau} = R_4 = I - \frac{h^2}{6} D_+ D_-, \quad R_{2\tau}^{(i)} = R_4^{(i)} = (I + \frac{h^2}{6} D_+ D_-)^{-1},$$

for solving Burgers' equation $(f(u) = u^2/2)$ with a stationary shock (s = 0). An explicit 3rd-order Runge-Kutta method has been used to solve a time dependent problem in a fixed coordinate system. Thus, the shock speed s does not appear explicitly in the equations. As initial data we have taken u(x,0) = -x, which should result in a stationary shock at the origin for $t \ge 1$. Furthermore, $u_L = 1$ and $u_R = -1$. From proposition 3.1 it follows that choosing ε according to eq. (16), i. e., $\varepsilon = 1/4$, should result in a one-point shock.

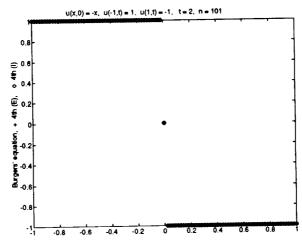


Fig. 1: One-Point Shock, 4th-order Explicit (+) and Implicit (o), $\varepsilon = 1/4$

Below is the result when the viscous terms are turned on only in a neighborhood of the shock. The viscosity is turned on and off by the switch defined by eq. (57). We also verify the theoretical results for the two-point shock. The coefficient ε is then given by eq. (22), that is, $\varepsilon = 3/8$.

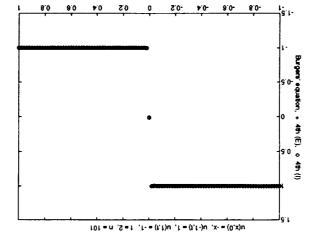


Fig. 2: One-Point Shock, 4th-order Explicit (+) and Implicit (0), $\epsilon=1/4$, Local Viscosity

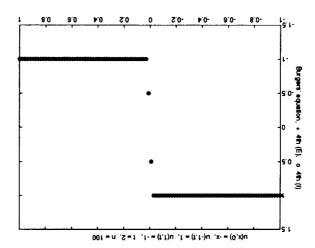


Fig. 3: Two-Point Shock, 4th-order Explicit (+) and Implicit (0), $\epsilon=3/8$

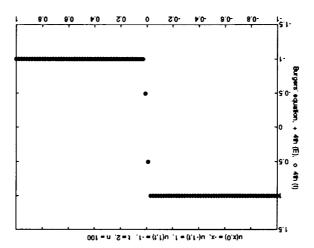


Fig. 4: Two-Point Shock, 4th-order Explicit (+) and Implicit (o), $\varepsilon = 3/8$, Local Viscosity

We now proceed to case where the shock is non-stationary. Again we compute in a fixed coordinate system using the factorized viscosity of section 3.1. Thus, the theory developed in the previous sections does not apply directly. It is still interesting to see how well this principle of introducing viscosity fares in practice. Indeed, it turns out that the viscosity coefficient ε obtained through linearization (26) works better in this case. In all of the following numerical experiments we have used the adaptive switch (57) to turn on viscosity locally around the shock; $u(x,0) = u_L$, x < 0, and $u(x,0) = u_R$, x > 0; $u_L = 2$, $u_R = 0$. Hence $\varepsilon = 1/2$. The solutions have been plotted at t = 1/2.

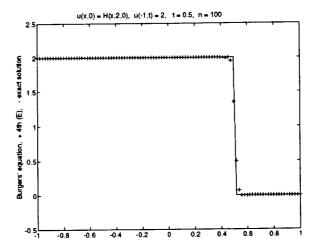


Fig. 5: Moving Shock, 4th-order Explicit, $\varepsilon = 1/2$

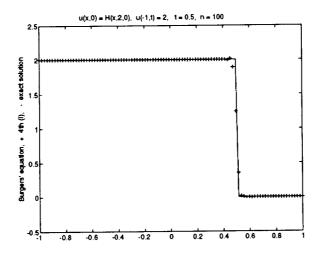


Fig. 6: Moving Shock, 4th-order Implicit, $\varepsilon = 1/2$

Next we employ the viscosity based on perturbation analysis as described in section 3.2. The data is the same as in the previous examples. The viscosity is now given by eq. (47), i. e., $\varepsilon_1 = 1/3$, $\varepsilon_2 = -1/12$. We also give two examples of the averaging technique of section 3.3.

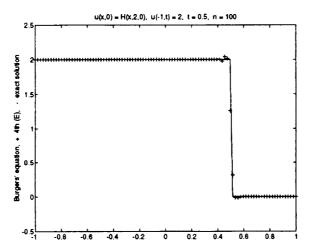


Fig. 7: Moving Shock, 4th-order Explicit, $\varepsilon_1=1/3,\,\varepsilon_2=-1/12$

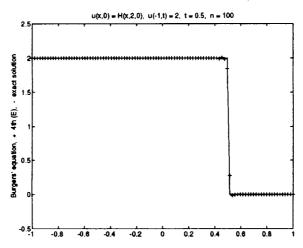


Fig. 8: Moving Shock, 4th-order Explicit, Averaging Viscosity

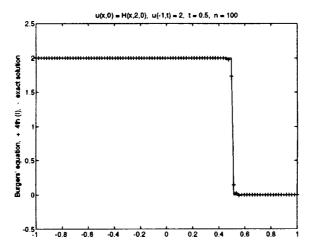


Fig. 9: Moving Shock, 4th-order Implicit, Averaging Viscosity

We conclude this section by showing two 4th-order computations where we have solved the linear advection equation $u_t + u_x = 0$ by means of the hybrid scheme (61). In the first example we have used $\varepsilon = 1/2$ and k = h. The switch r_j has been set to one at every grid point. The hybrid scheme is thus equivalent to the method of characteristics. In the second example $\varepsilon = 1/2$ and k = 0.9h; the switch r_j is now turned on adaptively. This implies that the numerical method should behave as an approximate upwind scheme near the discontinuity. The solutions have been plotted at t = 1/2.

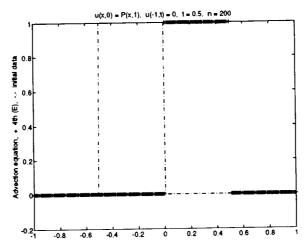


Fig. 10: Propagation of a Discontinuity, 4th-order Explicit (+), $-\cdot$ Initial Data, k=h

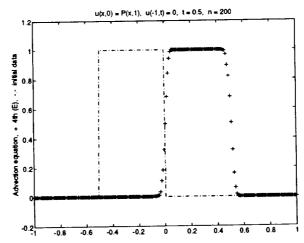


Fig. 11: Propagation of a Discontinuity, 4th-order Explicit (+), $-\cdot-$ Initial Data, k=0.9h

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