

High-Resolution Monotone Schemes Based on Quasi-Characteristics Technique

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In this article, we consider a new technique that allows us to overcome the well-known restriction of Godunov's theorem. According to Godunov's theorem, a second-order explicit monotone scheme does not exist. The techniques in the construction of high-resolution schemes with monotone properties near the discontinuities of the solution lie in choosing of one of two high-resolution numerical solutions computed on different stencils. The criterion for choosing the final solution is proposed. Results of numerical tests that compare with the exact solution and with the numerical solution obtained by the first-order monotone scheme are presented. © 2001 John Wiley & Sons, Inc. Numer Methods Partial Differential Eq 17: 262–276, 2001

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I. INTRODUCTION

It is well known that, according to Godunov's famous theorem, second-order explicit monotone schemes do not exist. But the problem of constructing high-resolution schemes with monotone properties near the discontinuities of the solution is the focus of much research in Computational Fluid Dynamics. There are currently two principal approaches to resolve this problem. The first consists of lowering the approximation order near the discontinuities of the solution. For instance, one can apply the first-order monotone schemes instead of the second-order scheme only in narrow regions, where the discontinuities of the solutions arise. Such schemes are known as hybrid schemes. In fact, most of the modern high-resolution schemes [1, 2] are of this type, because they implicitly set a restriction on coefficients lowering the order of approximation in zones where the discontinuities of the solution could arise. The second approach consists in the application of different high-resolution schemes of the same order defined on different stencils. Usually, such different stencils should be chosen implicitly, and only a careful analysis of the appropriate algorithm allows one to establish that the scheme is of the above-mentioned family.

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In this article, we consider the problem of constructing the second-order monotone schemes by a combination of two different second-order quasi-characteristics schemes. The heuristic criterion based on the theoretical estimation of the average value of the governing equation operator with respect to the grid cell is proposed for choosing the final solution among two suitable solutions of the second-order approximation. Some results of the numerical tests are presented. These results show that such an approach allows us to successfully construct monotone solutions of problems with discontinuities. A comparison of our numerical results with the exact solution and with the numerical solution computed by the first-order monotone scheme is also presented.

II. QUASI-CHARACTERISTICS SCHEMES

In this section, we present a short introduction to the theory of quasi-characteristics schemes, following [3].

Let us consider a Cauchy problem for the transport equation with respect to two independent variables:

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad -\infty < x < +\infty, \quad 0 < t \leq T; \quad (2.1)$$

$$u(x, 0) = u_0(x). \quad (2.2)$$

Here $u = u(x, t)$ is a searching function, and $a = a(x, t, u, \frac{\partial u}{\partial x})$, and $u_0(x)$ are known functions.

Let us denote $v = \frac{\partial u}{\partial x}$ and introduce any supplementary arbitrary function $b = b(x, t, u, \frac{\partial u}{\partial x})$. Then we can rewrite the governing equation in the equivalent form as a system of two equations with respect to unknown functions u and v :

$$\frac{\partial u}{\partial t} + (a + b) \frac{\partial u}{\partial x} = bv, \quad (2.3)$$

$$v = \frac{\partial u}{\partial x}. \quad (2.4)$$

Let b be equal to b_1 . In this case, we could choose a manifold

$$\frac{dx}{dt} = a + b_1, \quad (2.5)$$

on which the following condition is satisfied:

$$\frac{du}{dt} = b_1 v. \quad (2.6)$$

Here $\frac{du}{dt}$ is a total derivative of the function u with respect to t .

Let b be equal to b_2 . In this case, we could choose another manifold

$$\frac{dx}{dt} = a + b_2, \quad (2.7)$$

on which the following condition is satisfied:

$$\frac{du}{dt} = b_2 v . \tag{2.8}$$

Equations (2.5)–(2.8) are the expanded characteristic form of the transport Eq. (2.1). This system is also a closed system with respect to unknown functions u and v , and is also equivalent to the system (2.3–2.4), which is again equivalent to Eq. (2.1). Equations (2.5) and (2.7) define expanded characteristic manifolds.

Based on the expanded characteristic form, it is possible to construct a numerical scheme similar to the well-known numerical scheme of the method of characteristics in the 2-D case. Choosing arbitrary functions b_1 and b_2 in constructing the scheme should be done for the suitable numerical realization manifolds, for instance, coordinate or nodal grid lines. We shall call such grid lines *quasi-characteristics*, because, if these lines coincide with characteristics of the governing equation, then the expanded characteristics form of the governing equation on these lines automatically turns into the normal characteristic form.

Now let us consider a finite difference uniform grid with steps h and τ such that $x_j = jh$, $t_n = n\tau$, where $j = 0, \pm 1, \pm 2, \dots$; $n = 0, 1, 2, \dots, N = T/\tau$ in a plane (x, t) . Further, we shall suppose that $a = \text{const} > 0$ for simplicity. One fragment of the grid under consideration is shown in Fig. 1. The dash lines in this figure show the characteristics of the governing transport equation.

Let us suppose that points $m_-, m_0,$ and m_+ lie at the known layer $t = t_n$ (we know all searching functions at this layer) and points $n_-, n_0,$ and n_+ lie at the new layer $t = t_n + \tau$, where we want to compute the values of the searching grid functions.

Let us choose $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = -a$. Then the manifolds described by Eqs. (2.5) and (2.7) are equations of two families of grid lines. So the first family consists of the lines parallel to the grid line m_-n_0 , and the second consists of the lines parallel to the grid line m_0n_+ . Integrating Eqs. (2.6) and (2.8) along these lines by the Euler method of the second-order approximation, we obtain the following explicit scheme of the second-order approximation:

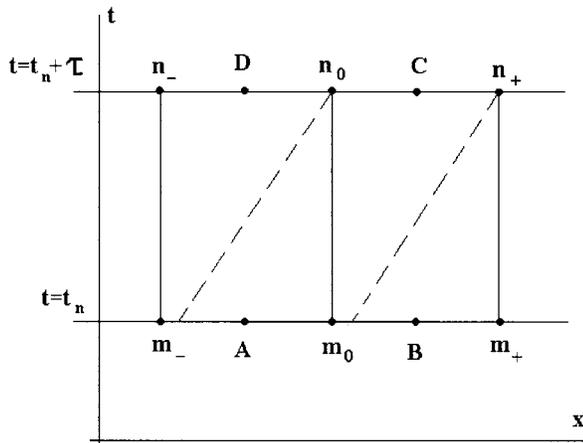


FIG. 1. The grid fragment.

$$\left. \begin{aligned} u(n_0) - u(m_-) &= \frac{1}{2}h(1-k)[v(m_-) + v(n_0)] , \\ u(n_0) - u(m_0) &= -\frac{1}{2}hk[v(m_0) + v(n_0)] . \end{aligned} \right\} \quad (2.9)$$

Here $k = \frac{a\tau}{h}$ is a Courant number.

Let us denote $\delta u = u(n_0) - u(m_0)$ and $\delta v = v(n_0) - v(m_0)$. Here δu and δv are gains of searching functions at the points of the new layer.

Solving system (2.9) with respect to δu and δv , we obtain the following explicit formulas for the evaluation of searching grid functions at the new layer:

$$\left. \begin{aligned} \delta u &= k[u(m_-) - u(m_0)] + \frac{1}{2}hk(k-1)[v(m_0) - v(m_-)] , \\ \delta v &= -\frac{2}{h}[u(m_-) - u(m_0)] + (k-1)[v(m_0) + v(m_-)] - 2kv(m_0) . \end{aligned} \right\} \quad (2.10)$$

If we choose $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = (-\frac{h}{\tau} - a)$, then, as before, the manifold described by Eqs. (2.5) corresponds to the family of lines parallel to the grid line m_-n_0 , but the manifold described by Eqs. (2.7) corresponds to the family of lines parallel to the grid line m_+n_0 . The appropriate approximation of Eqs. (2.6) and (2.8) along these lines are as follows:

$$\begin{aligned} u(n_0) - u(m_-) &= \frac{1}{2}h(1-k)[v(m_-) + v(n_0)] , \\ u(n_0) - u(m_+) &= -\frac{1}{2}h(1+k)[v(m_+) + v(n_0)] . \end{aligned}$$

We could also rewrite these formulas in terms of gains of searching grid functions as follows:

$$\left. \begin{aligned} \delta u + \frac{1}{2}(k-1)h\delta v &= u(m_-) - u(m_0) + \frac{1}{2}h(1-k)[v(m_-) + v(m_0)] , \\ \delta u + \frac{1}{2}(k+1)h\delta v &= u(m_+) - u(m_0) - \frac{1}{2}h(1+k)[v(m_+) + v(m_0)] . \end{aligned} \right\} \quad (2.11)$$

Solving system (2.11) with respect to δu and δv , we obtain another explicit scheme of the second-order approximation:

$$\left. \begin{aligned} \delta u &= \frac{1}{2}[(1-k)u(m_+) - 2u(m_0) + (1+k)u(m_-)] \\ &\quad - \frac{1}{4}h(1-k^2)[v(m_+) - v(m_-)] , \\ \delta v &= \frac{1}{h}[u(m_+) - u(m_-)] - \frac{1}{2}\{(1-k)[v(m_0) + v(m_-)] \\ &\quad + (1+k)[v(m_0) + v(m_+)]\} . \end{aligned} \right\} \quad (2.12)$$

III. SELECTION CRITERION

Both schemes (2.10) and (2.12) are of the second-order approximation. It is well known that, if we directly apply these schemes to the problems with discontinuous solutions, then the resulting numerical solutions have high-frequency spurious oscillations near the discontinuities. In Refs. 3 and 4, it was shown that using a combination of schemes (2.10) and (2.12) instead of one scheme

alone on the fixed stencil allows us to obtain the monotone solution without high-frequency spurious oscillations near the discontinuities. To provide a monotone solution in this approach, in each nodal point of the new layer two solutions by schemes (2.10) and (2.12) are evaluated, and we choose one of them, according to a *special criterion*, as a final solution. The criterion proposed in the cited articles is based on the estimation of the average value of the differential operator of the governing equation in the cell of finite difference grid. Unfortunately, this criterion is very complicated and not suitable for parallel computations, because it takes into account the history of computations at the new layer. Further, we suggest a simpler criterion suitable for the parallel computations. This criterion is also based on the estimation of the average value of the differential operator of the governing equation in the grid cell, but it is not connected with the history of the computations at the new layer and, thus, has a local character.

Let us consider the average value $M_L(u)$ of the governing differential operator $L(u) = \frac{\partial u}{\partial t} + \frac{\partial(au)}{\partial x}$ in any region D with boundary ∂D . This value is defined by

$$M_L(u) = \frac{\int_D L(u) dxdt}{\int_D dxdt} .$$

Here we assume that function $u(x, t)$ exists, is sufficiently smooth in $D + \partial D$, and its first derivatives are also smooth. Then we have

$$M_L(u) = \frac{\int_D (\frac{\partial u}{\partial t} + \frac{\partial(au)}{\partial x}) dxdt}{\int_D dxdt} = \frac{\oint_{\partial D} (-udx + audt)}{\int_D dxdt} . \tag{3.1}$$

Choosing D as an elementary cell of finite difference grid with vertexes $A, B, C,$ and D (see Fig. 1), where $A = \frac{1}{2}(m_- + m_0), B = \frac{1}{2}(m_+ + m_0), C = \frac{1}{2}(n_+ + n_0), D = \frac{1}{2}(n_0 + n_-)$, and, evaluating integrals in (3.1) over this region, we obtain

$$\int_D dxdt = h\tau , \quad \oint_{\partial D} (-udx + audt) = -\int_A^B udx + \int_B^C audt + \int_C^D udx - \int_D^A audt .$$

We evaluate integrals on the right-hand side of the last formula by the simple quadrature formula of rectangles. Thus, we obtain

$$\oint_{\partial D} (-udx + audt) = -\frac{u_A + u_B}{2}h + a\frac{u_B + u_C}{2}\tau + \frac{u_D + u_C}{2}h - a\frac{u_A + u_D}{2}\tau + O(h_*^3) .$$

Here $h_* = \max\{h, \tau\}$.

If we present u_A and u_B by the following second-order approximation formulas

$$u_A = \frac{u(m_-) + u(m_0)}{2} + O(h^2) , \quad u_B = \frac{u(m_0) + u(m_+)}{2} + O(h^2) ,$$

then we obtain

$$\oint_{\partial D} (-udx + audt) = -\frac{u(m_-)+u(m_0)}{4}(h + a\tau) - \frac{u(m_+)+u(m_0)}{4}(h - a\tau) + \frac{a\tau}{2}(u_C - u_D) + \frac{1}{2}h(u_C + u_D) + O(h_*^3).$$

Thus, we obtain

$$\begin{aligned} \oint_{\partial D} (-udx + audt) &= -\frac{h}{4}\{(1+k)[u(m_-) + u(m_0)] \\ &+ (1-k)[u(m_+) + u(m_0)]\} + \frac{1}{2}kh^2v(n_0) + hu(n_0) + O(h_*^3). \end{aligned}$$

In the deduction of the last formula, the following approximations have been used:

$$u_C - u_D = v(m_0)h + O(h^3), \quad \frac{u_C + u_D}{2} = u(n_0) + O(h^2).$$

Therefore, the average value of the considering differential operator becomes

$$\begin{aligned} M_L(u) &= \frac{1}{\tau}\{\frac{1}{2}hk[v(m_0) + \delta v] + u(m_0) + \delta u \\ &- \frac{1}{4}(1+k)[u(m_0) + u(m_-)] - \frac{1}{4}(1-k)[u(m_0) + u(m_+)]\} + O(h_*). \end{aligned}$$

At the first stage of our algorithm, we compute gains of searching functions δu and δv at each nodal point of the new layer by schemes (2.10) and (2.12), and then choose the final pair of such functions so that the absolute value of the principal part of $M_L(u)$,

$$\begin{aligned} &|\frac{1}{2}hk[v(m_0) + \delta v] + u(m_0) + \delta u - \frac{1}{4}(1+k)[u(m_0) + u(m_-)] \\ &- \frac{1}{4}(1-k)[u(m_0) + u(m_+)]|, \end{aligned} \tag{3.2}$$

is minimized! We call this Scheme I.

IV. SCHEME WITH APPROXIMATION OF OUTWARD DERIVATIVES AT THE MIDDLE LAYER

In the previous section, we have considered the scheme with approximation of the outward derivative v with respect to the quasi-characteristic by its grid values taken at the data and at the computing layers. If we use the Euler method to evaluate this derivative at the middle layer $t = t_n + \frac{\tau}{2}$, then we obtain a second-order approximation scheme. Such a scheme was proposed and considered in [5-7]. In this way, we take $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = (-\frac{h}{\tau} - a)$ and approximate Eqs. (2.6) and (2.8) with the second-order Euler approximation error along the quasi-characteristics parallel to m_-n_0 and m_+n_0 grid lines. As a result, we obtain the following expressions:

$$\left. \begin{aligned} u(n_0) - u(m_-) &= \tau(\frac{h}{\tau} - a)v(t_n + \frac{\tau}{2}, x_0 - \frac{h}{2}), \\ u(n_0) - u(m_+) &= -\tau(\frac{h}{\tau} + a)v(t_n + \frac{\tau}{2}, x_0 + \frac{h}{2}). \end{aligned} \right\} \tag{4.1}$$

Here and hereafter, we use the notation $x_i = x_{m_i}$, ($i = +, 0, -$).

For an approximation of the outward derivative $v(t_n + \frac{\tau}{2}, x)$, the following formulas are used:

$$\left. \begin{aligned} v(t_n + \frac{\tau}{2}, x) &= v(t_n + \frac{\tau}{2}, x_0) + \frac{(x-x_0)}{h}W(m_0), \\ W(m_0) &= \frac{u(m_+) - 2u(m_0) + u(m_-)}{h}. \end{aligned} \right\} \quad (4.2)$$

Then

$$v(t_n + \frac{\tau}{2}, x_0 \pm \frac{h}{2}) = v(t_n + \frac{\tau}{2}, x_0) \pm \frac{1}{2}W(m_0). \quad (4.3)$$

Substitution of (4.3) into (4.1) and elimination of $v(t_n + \frac{\tau}{2}, x_0)$ yields the following explicit second-order scheme for evaluating $u(n_0)$ at the new layer:

$$u(n_0) = \frac{1}{2}[(1+k)u(m_-) + (1-k)u(m_+) - (1-k^2)hW(m_0)], \quad (4.4)$$

or

$$\delta u = \frac{1}{2}[(1+k)u(m_-) - 2u(m_0) + (1-k)u(m_+) - (1-k^2)hW(m_0)]. \quad (4.5)$$

If we want to use the technique described in the previous section for the construction of monotone solutions for problems with discontinuities, then we must construct the second scheme for comparison. Of course, it seems simple to consider the appropriate scheme, corresponding to choosing $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = -a$, as in Section II. But, in this case, direct evaluations show that substitution of the approximation of the outward derivatives at the middle layer,

$$v(t_n + \frac{\tau}{2}, x_0 - \frac{h}{2}) = v(t_n + \frac{\tau}{2}, x_0) - \frac{1}{2}W(m_0)$$

into approximations of Eqs. (2.6) and (2.8) gives

$$\left. \begin{aligned} u(n_0) - u(m_-) &= \tau(\frac{h}{\tau} - a)v(t_n + \frac{\tau}{2}, x_0 - \frac{h}{2}), \\ u(n_0) - u(m_0) &= -\tau av(t_n + \frac{\tau}{2}, x_0) \end{aligned} \right\} \quad (4.6)$$

and this also yields the formulas (4.4–4.5) for evaluation of $u(n_0)$ at the point n_0 at the new layer. Therefore, to construct the second scheme for the comparison of solutions, we take another approximation of the outward derivative at the middle layer. Let us take an approximation with a shift as follows:

$$\left. \begin{aligned} v(t_n + \frac{\tau}{2}, x) &= v(t_n + \frac{\tau}{2}, x_0 - h) + \frac{(x-x_0+h)}{h}W(m_-), \\ W(m_-) &= \frac{u(m_0) - 2u(m_-) + u(x_0-h)}{h}. \end{aligned} \right\} \quad (4.7)$$

Then we have

$$\left. \begin{aligned} v(t_n + \frac{\tau}{2}, x_0 - \frac{h}{2}) &= v(t_n + \frac{\tau}{2}, x_0 - h) + \frac{1}{2}W(m_-), \\ v(t_n + \frac{\tau}{2}, x_0) &= v(t_n + \frac{\tau}{2}, x_0 - h) + W(m_-). \end{aligned} \right\} \quad (4.8)$$

Substituting (4.8) into (4.6) and eliminating $v(t_n + \frac{\tau}{2}, x_0 - h)$ yields the following formulas for the second scheme:

$$u(n_0) = (1 - k)u(m_0) + ku(m_-) - \frac{1}{2}k(1 - k)hW(m_-), \quad (4.9)$$

or

$$\delta u = -k[u(m_0) - u(m_-)] - \frac{1}{2}k(1 - k)hW(m_-). \quad (4.10)$$

Now we consider the problem of choosing the final solution among two preliminary evaluated solutions (4.4–4.5) and (4.9–4.10).

We again consider the condition (3.2) as a selection criterion of the possible solutions evaluated by schemes (4.4–4.5) and (4.9–4.10). But, in this case, the outward derivative v in the first term of the formula (3.2) is not available. But, because the order of this term is about $O(h_*)$ while all other terms are about $O(1)$, we can omit the first term in (3.2) without losing significance. Thus, we obtain the following criterion to minimize:

$$\left| u(m_0) + \delta u - \frac{1}{4}(1 + k)[u(m_0) + u(m_-)] - \frac{1}{4}(1 - k)[u(m_0) + u(m_+)] \right| - > \min.$$

We call the scheme proposed here Scheme II.

V. NUMERICAL TESTS

Because we have presented only the heuristic speculations about the construction of the selection criteria, we need to provide numerical tests of our schemes. We consider a numerical solution of the Cauchy problem for the governing transport equation with the coefficient $a = 0.9$ and with the discontinuous initial data $u_0(x)$ described by the following piecewise constant function:

$$u_0(x) = \begin{cases} 1, & \text{if } x \leq 0.6; \\ (1 - \frac{i}{7}) & \text{if } 0.6 \cdot i < x \leq 0.6 \cdot (i + 1), \quad i = 1, 2, \dots, 6; \\ 0 & \text{if } x > 4.2. \end{cases}$$

This problem has an exact wave type analytical solution: $u(x, t) = u_0(x - at)$. We shall take it for the comparison with the numerical solutions.

We note that we should set an additional initial condition for function v only for Scheme I. We set this function identically equal to zero at the initial layer, meaning that $v(x, 0) = 0$. All presented numerical results are computed on the uniform grid with the spatial step $h = 0.05$. Results of computations are presented for the following values of the time-step and Courant number, respectively: (1) $\tau = 0.05$ ($k = 0.9$), (2) $\tau = 0.04$ ($k = 0.72$), and (3) $\tau = 0.025$ ($k = 0.45$).

Also, we shall compare our numerical results of the second-order approximation with numerical results obtained by the very popular left-angle monotone scheme of the first-order approximation, which is an analogy of the well-known Godunov scheme for considering the initial problem. This scheme corresponds to the first two terms of formulas (4.9–4.10), namely:

$$u(n_0) = (1 - k)u(m_0) + ku(m_-), \quad (5.1)$$

or

$$\delta u = -k[u(m_0) - u(m_-)]. \quad (5.2)$$

We shall call this Scheme L.

We shall provide comparison of the solutions for functions $u(x, t)$ and $v(x, t)$ for $t = 2$ and $t = 5$, and, as a derivative of the exact solution, we shall take the following grid function $v_j = (\tilde{u}_{j+1} - \tilde{u}_j)/h$, where $\tilde{u}_j = u_0(x_j - at)$. For Scheme II, we evaluate v_j as $v_j = (u_{j+1} - u_j)/h$. In the following figures, the first picture corresponds to the function $u(x, t)$ and the second to

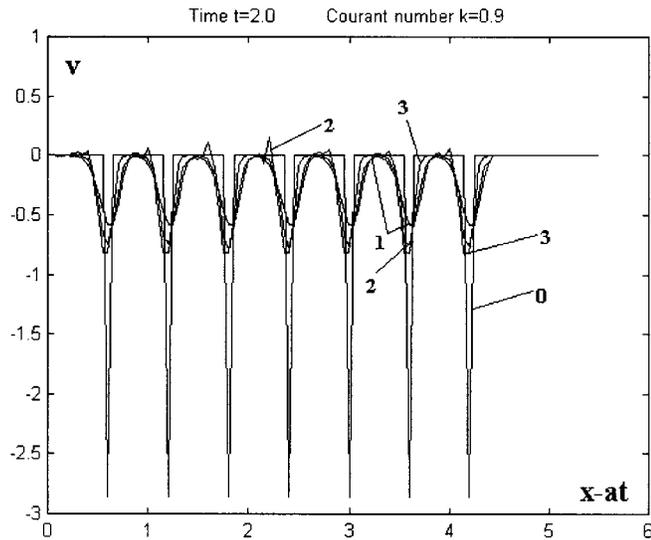
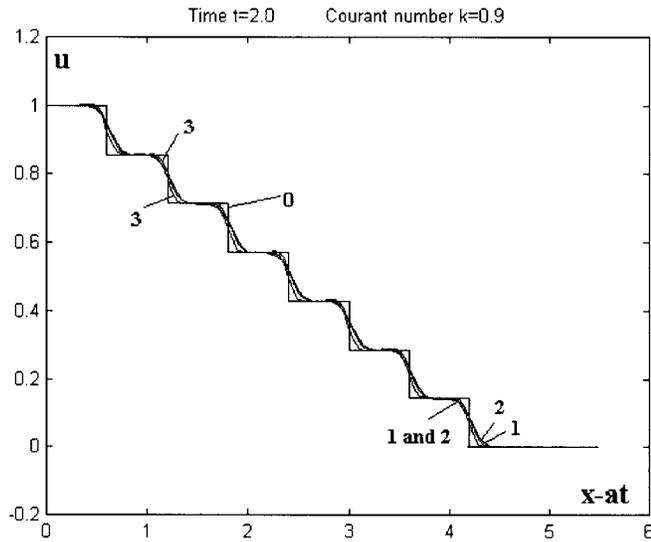


FIG. 2. Plots of u and v for $t = 2$ and $k = 0.9$.

the function $v(x, t)$. It is very important to analyze the function $v_j(x, t)$, because, as shown in [3], even high-resolution schemes of the fourth order could not properly capture this function and give the same result as the first-order scheme.

Figure 2 shows the comparison of numerical results and analytical solution for $t = 2$ and $k = 0.9$, Fig. 3 corresponds to $t = 5$ and $k = 0.9$, Fig. 4 to $t = 2$ and $k = 0.72$, Fig. 5 to $t = 5$

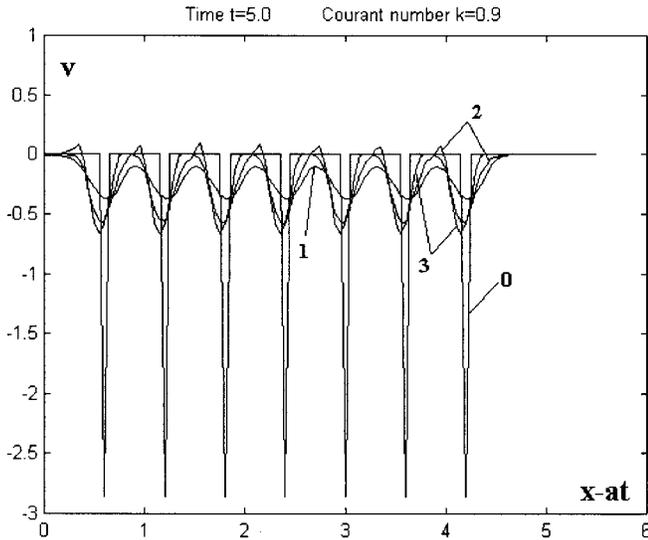
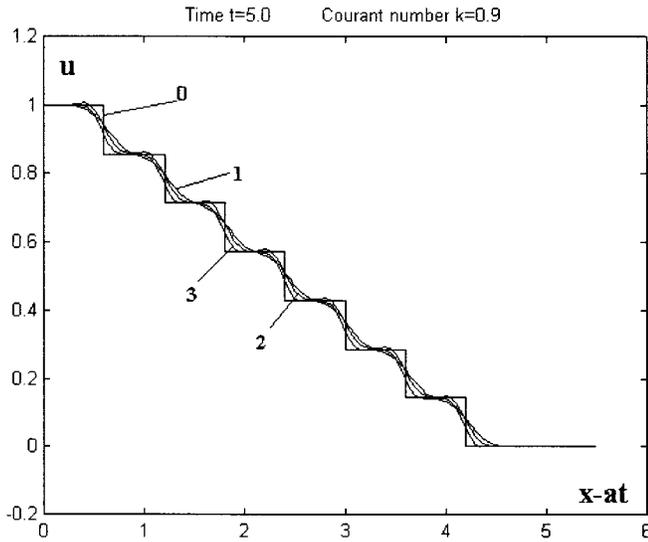


FIG. 3. Plots of u and v for $t = 5$ and $k = 0.9$.

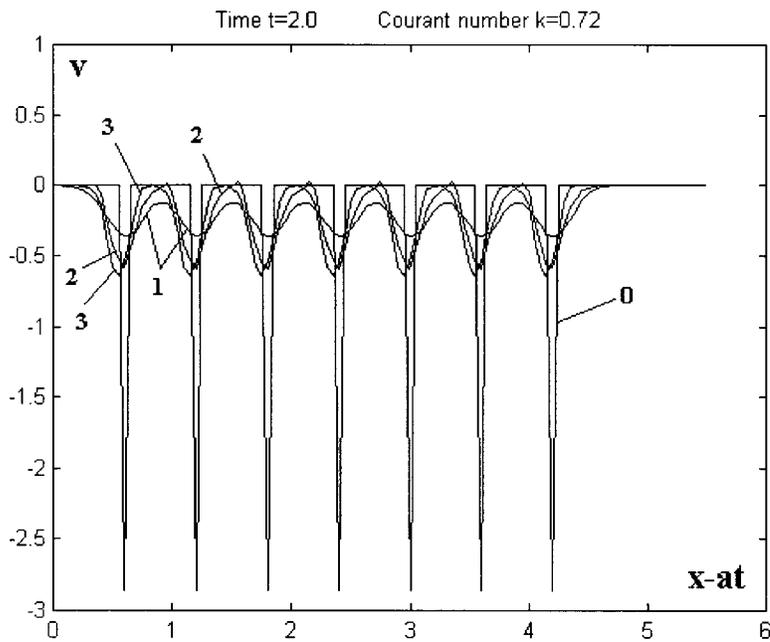
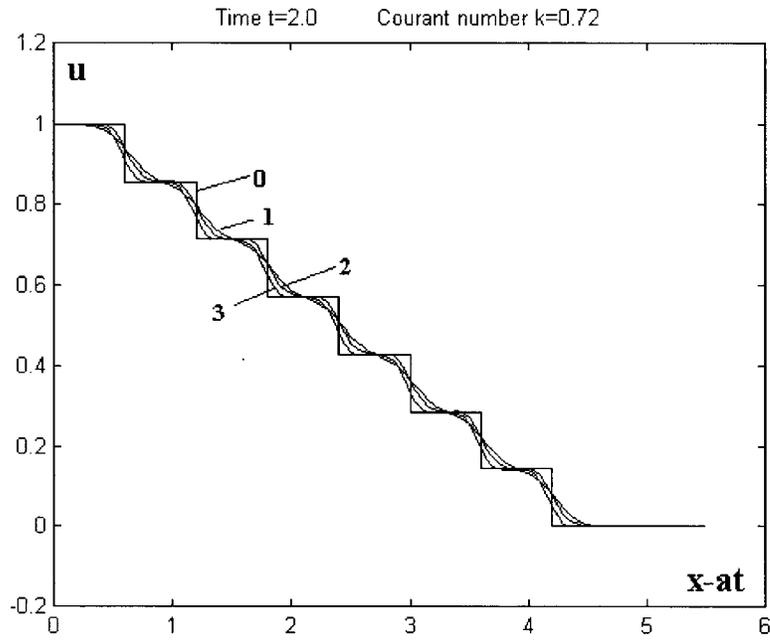


FIG. 4. Plots of u and v for $t = 2$ and $k = 0.72$.

and $k = 0.72$, Fig. 6 to $t = 2$ and $k = 0.45$, and Fig. 7 to $t = 5$ and $k = 0.45$. In these figures, Line 0 corresponds to the analytical solution, Line 1 corresponds to the solutions computed by

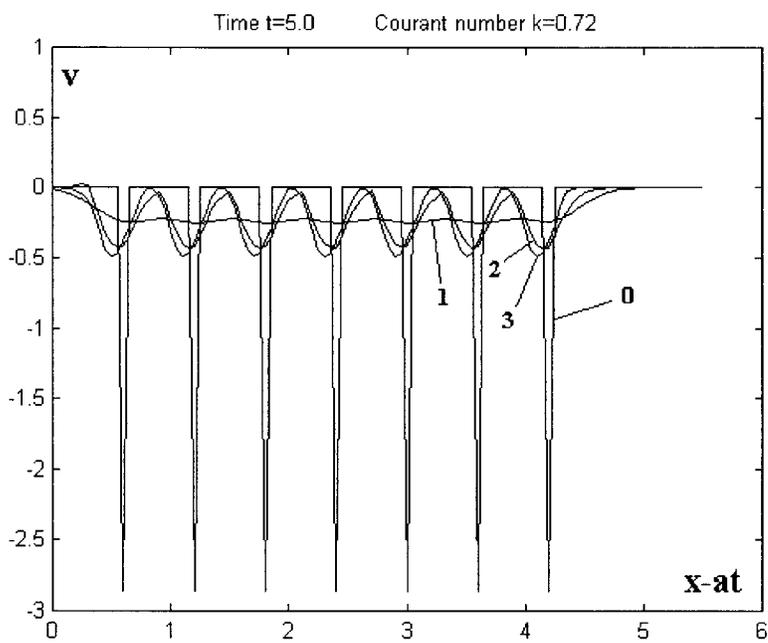
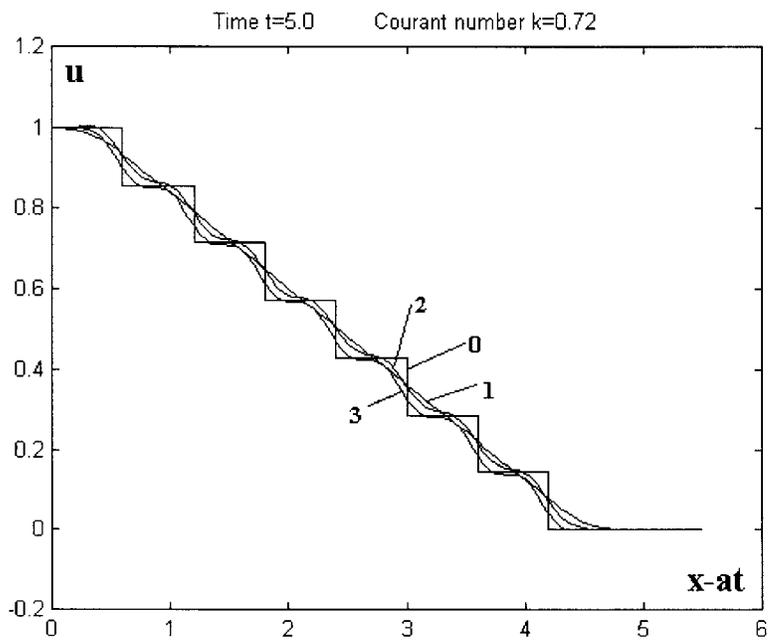


FIG. 5. Plots of u and v for $t = 5$ and $k = 0.72$.

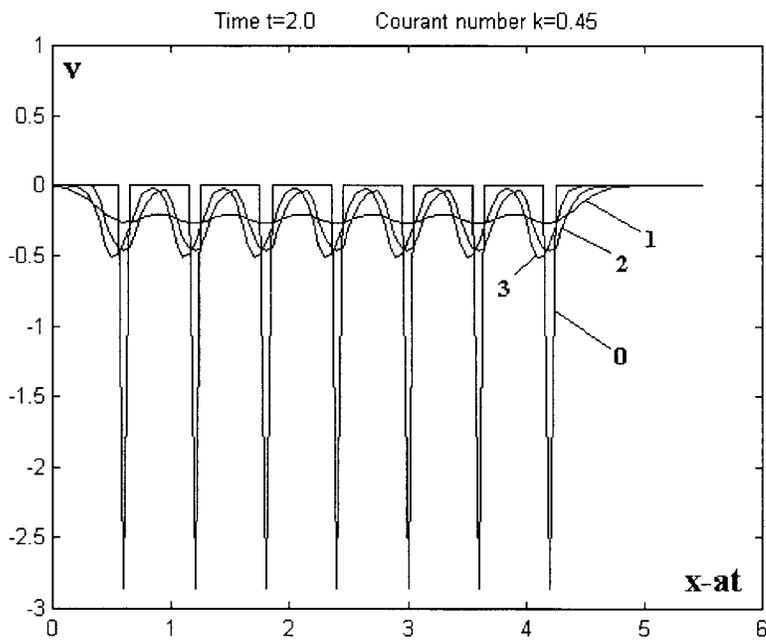
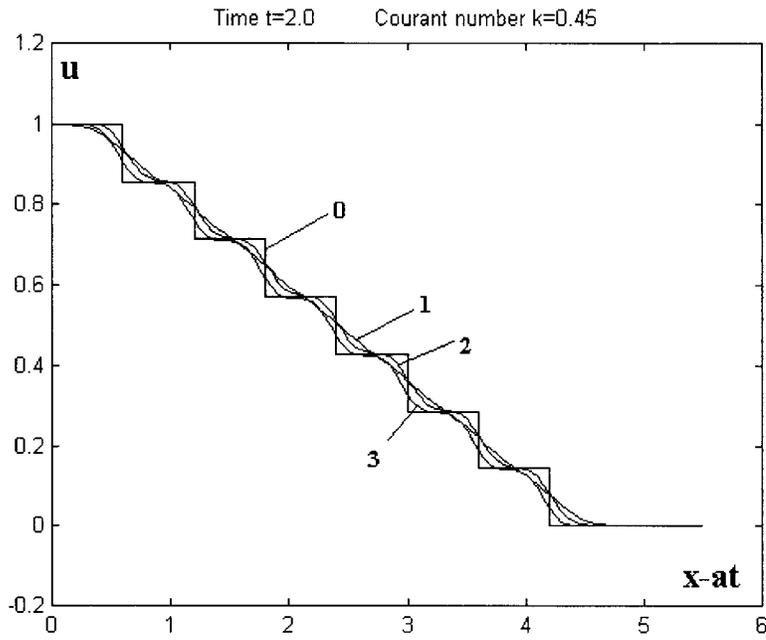


FIG. 6. Plots of u and v for $t = 2$ and $k = 0.45$.

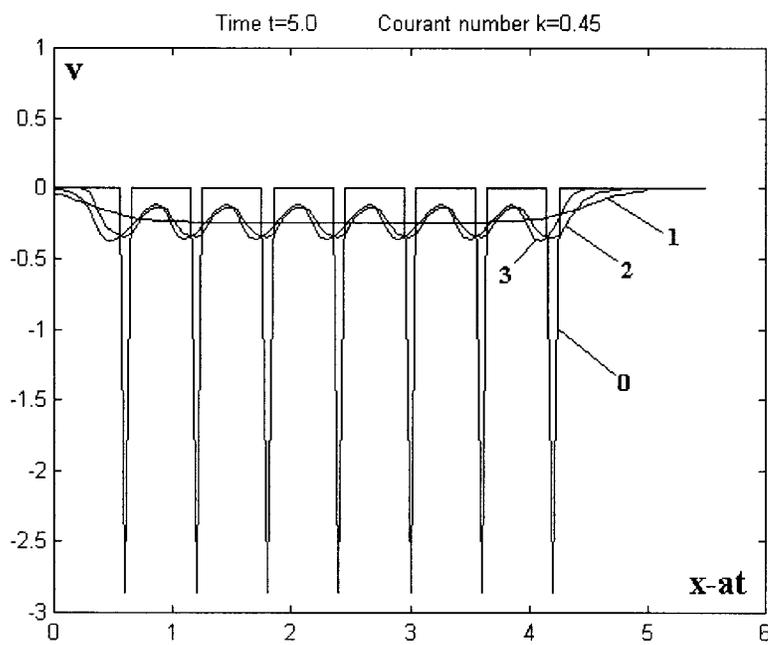
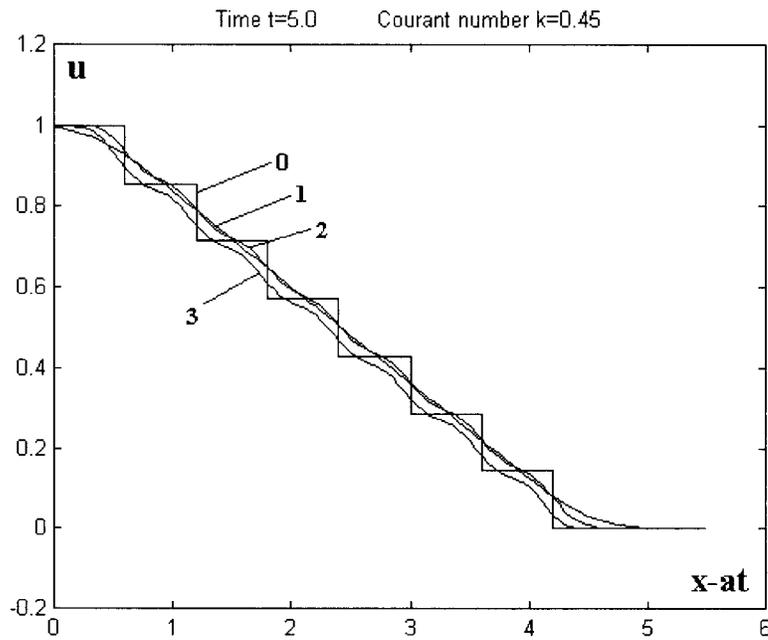


FIG. 7. Plots of u and v for $t = 5$ and $k = 0.45$.

Scheme L, Line 2 corresponds to the solutions computed by Scheme I, and Line 3 corresponds to the solutions computed by Scheme II.

These results show that solutions obtained by Scheme I are almost everywhere monotonous, except very small regions in the case where $k = 0.9$ and for $k = 0.72$ and $k = 0.45$ (they are practically strictly monotonous). Solutions computed by Scheme II are strictly monotonous for all taken Courant numbers. According to the presented results, we could see that in the case where $k = 0.9$, all schemes catch the peculiarities of the solutions for $t = 2$ and $t = 5$. In the case where $k = 0.72$ and $k = 0.45$, Schemes I and II catch the peculiarities of the solutions for $t = 2$ and $t = 5$, but Scheme L of the first-order approximation describes the peculiarities of the solutions only for $k = 0.72$ and $t = 2$, and practically could not describe the character of the solutions for $k = 0.72$, $t = 5$, and for $k = 0.45$ in the cases where $t = 2$ and $t = 5$. Computational results also show that Scheme II gives sharper shocks than Scheme I in all cases, and both these schemes give essentially sharper shocks than Scheme L of the first-order approximation – especially in case of small Courant numbers. The best results are obtained by Scheme II in all ranges of the considered parameters.

VI. CONCLUSIONS

The numerical schemes considered here are constructed as a combination of two different second-order quasi-characteristics schemes, switching according to the proposed heuristic criteria. These schemes are suitable for parallel computations that allow us to successfully simulate practically monotone solutions of problems with discontinuities. In comparison with the first-order approximation monotone scheme, these schemes give essentially sharper shocks.

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