Trends in Mathematics
Information Center for Mathematical Sciences
Volume 3, December 2000, Pages 51–59

INTRODUCTION IN QUASI-CHARACTERISTICS SCHEMES

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ABSTRACT. A survey of various quasi-characteristics numerical schemes is presented. The analysis of schemes is provided on Cauchy problem for the transport equation. For solution of initial value hyperbolic problems with discontinuities two approaches are considered. The first approach consists in choosing of final solution among two high order solutions computed on different stencils and the second consists in using of hybrid modification of considering schemes.

1. INTRODUCTION

Numerical schemes of the method of characteristics have a more higher precision in comparing with other approaches because they are based on characteristic properties of governing equations of hyperbolic type. However in modern practice these schemes are not widely used due their complexity especially in 3D case. Here we consider some new types of quasi-characteristics schemes developed in recent years [1-7]. These schemes are based on approximation of the governing hyperbolic equations written in expanded characteristic form along quasi-characteristics. They are a generalization of well known backward characteristics schemes but don't include any interpolation procedures for redefinition of data on each layer orthogonal to the marching direction due approximation of governing equations in the expanded characteristic form along the quasi-characteristics (special grid lines forming a region containing characteristics of governing equations and lying at a short distance to characteristics). This significantly simplifies the realization of these schemes and also cuts a number of operations that respectively leads to the rising of precision of computations and makes these schemes very attractive in 3D case.

To date for computations of solutions with discontinuities two approaches in realization of quasi-characteristics schemes are proposed. In the first approach solutions on two different stencils are computed and the final solution is chosen according to the special criterion proposed in [1-2]. This criterion is obtained basing on consideration of the average value of the differential operator of governing equation with respect to finite difference cell. Unfortunately this criterion is very complicated because it takes into account a history of previous computations and its realization in 3D case was not provide to date. The second approach [3-5] consists in lowering of the order of approximation in narrow regions where discontinuities of solutions could arise. This approach is known a hybrid modification of quasi-characteristics schemes. It is more simple in comparing with the firs approach and it was realized in 3D case in [4,5,7,8] with success.

2000 *Mathematics Subject Classification.* 65M06, 65M25.
Key words and phrases. quasi-characteristics, monotone schemes, hybrid schemes.
Received July 31, 2000.

2. Expanded Characteristics Form of Governing Equation

To explain a principles of the quasi-characteristics methods we take into consideration a simple example of an initial value problem for the transport equation in 2D case

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \ , \qquad t > 0 \ , \ -\infty < x < +\infty \ , \qquad u(0,x) = g(x) \ . \tag{1}$$

Here $u(t,x)$ is a searching function, $a = const > 0$ and $g(x)$ is a known function.

The first step of the quasi-characteristics technique consists in transformation of the governing equation of (1) in the expanded characteristics form.

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

$$\frac{\partial u}{\partial t} + (a+b)\frac{\partial u}{\partial x} = bv, \tag{2}$$

$$v = \frac{\partial u}{\partial x} \ . \tag{3}$$

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

$$\frac{dx}{dt} = a + b_1 \ , \tag{4}$$

on which the following condition is satisfied

$$\frac{du}{dt} = b_1 v \ . \tag{5}$$

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

$$\frac{dx}{dt} = a + b_2 \ , \tag{6}$$

on which the following condition is satisfied

$$\frac{du}{dt} = b_2 v \ . \tag{7}$$

Equations (4-7) are expanded characteristic form of the transport equation (1). This system also is a closed system with respect to unknown functions u and v and also it is equivalent to the system (2-3) that is again equivalent to the equation (1). Equations (4) and (6) 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 2D case. Choosing arbitrary functions b_1 and b_2 in constructing the scheme should be done to provide approximation on the suitable for numerical realization manifolds, for instance, along coordinate or nodal grid lines. We shall call such nodal grid lines *quasi-characteristics*, because if these lines coincide with characteristics of governing equation, then the expanded characteristics form of governing equations on these lines automatically turns into the normal characteristic form.

3. Quasi-Characteristics Schemes

Now let us consider a finite difference uniform grid with steps h and τ such $x_j = jh$, $t_n = n\tau$, where $j = 0, \pm 1, \pm 2, ...;$ $n = 0, 1, 2, ..., N = T/\tau$ in a plane (x, t). One fragment of the grid under consideration is shown in Fig.1. The dash lines in this figure show the characteristics of the

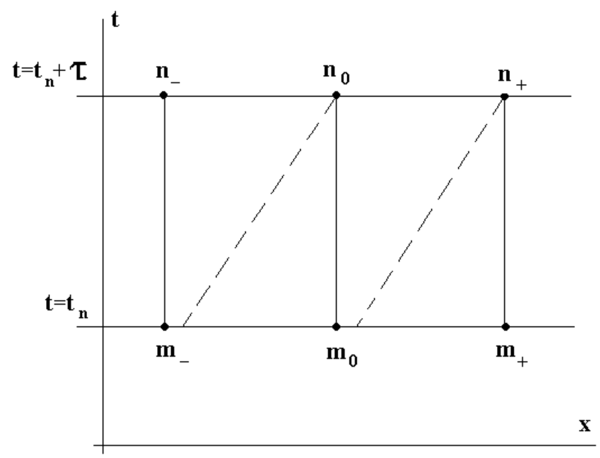

Fig.1. The grid fragment.

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 searching grid functions.

3.1. **Scheme with Half-Sum Approximiation of Outward Derivatives.** Let us choose $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = -a$. Then the manifolds described by equations (4) and (6) 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 $m_0 n_0$. Integrating equations (4) and (6) along these lines by the Euler method of the second order approximation we obtain the following explicit scheme of the second order approximation

$$\left.\begin{aligned} u(n_0) - u(m_-) &= \tfrac{1}{2}h(1-k)[v(m_-) + v(n_0)]\ , \\ u(n_0) - u(m_0) &= -\tfrac{1}{2}hk[v(m_0) + v(n_0)]\ . \end{aligned}\right\} \tag{8}$$

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 (5) with respect to δu and δv we obtain the following explicit formulas for the evaluation of searching grid functions at the new layer

$$\left.\begin{aligned} \delta u &= k[u(m_-) - u(m_0)] + \tfrac{1}{2}hk(k-1)[v(m_0) - v(m_-)]\ , \\ \delta v &= -\tfrac{2}{h}[u(m_-) - u(m_0)] + (k-1)[v(m_0) + v(m_-)] - 2kv(m_0)\ . \end{aligned}\right\} \tag{9}$$

If we choose $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = (-\frac{h}{\tau} - a)$, then as before the manifold described by the equation (4) corresponds to the family of lines parallel to the grid line m_-n_0, but the manifold described by the equation (6) corresponds to the family of lines parallel to the grid line m_+n_0. The appropriate approximations of equations (5) and (7) along these lines are as follows:

$$\left.\begin{aligned} u(n_0) - u(m_-) &= \tfrac{1}{2}h(1-k)[v(m_-) + v(n_0)] \ , \\ u(n_0) - u(m_+) &= -\tfrac{1}{2}h(1+k)[v(m_+) + v(n_0)] \ . \end{aligned}\right\} \tag{10}$$

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

$$\left.\begin{aligned} \delta u + \tfrac{1}{2}(k-1)h\delta v &= u(m_-) - u(m_0) + \tfrac{1}{2}h(1-k)[v(m_-) + v(m_0)] \ , \\ \delta u + \tfrac{1}{2}(k+1)h\delta v &= u(m_+) - u(m_0) - \tfrac{1}{2}h(1+k)[v(m_+) + v(m_0)] \ . \end{aligned}\right\} \tag{11}$$

Solving system (11) with respect to δu and δv we obtain another explicit scheme of the second order approximation

$$\left.\begin{aligned} \delta u = \tfrac{1}{2}[(1-k)u(m_+) - 2u(m_0) + (1+k)u(m_-)] - \\ \tfrac{1}{4}h(1-k^2)[v(m_+) - v(m_-)] \ , \\ \delta v = \tfrac{1}{h}[u(m_+) - u(m_-)] - \tfrac{1}{2}\{(1-k)[v(m_0) + v(m_-)] + \\ (1+k)[v(m_0) + v(m_+)]\} \ . \end{aligned}\right\} \tag{12}$$

The scheme considered above was investigated and proposed in [1-2]. In this scheme we need to compute and to storage in computer core the values of the supplementary variable $\frac{\partial u}{\partial x}$ in grid points.

3.2. **Scheme with Approximiation of Outward Derivatives at Middle Layer.** In the previous subsection 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 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 scheme was proposed in [3]. In this way we take $b_1 = (\frac{h}{\tau} - a)$ and $b_2 = (-\frac{h}{\tau} - a)$ and approximate equations (5) and (7) with the second order approximation error along the quasi-characteristics parallel to m_-n_0 and m_+n_0 grid lines. As a result we obtain two following expressions:

$$\left.\begin{aligned} u(n_0) - u(m_-) &= \tau(\tfrac{h}{\tau} - a)v(t_n + \tfrac{\tau}{2}, x_0 - \tfrac{h}{2}) \ , \\ u(n_0) - u(m_+) &= -\tau(\tfrac{h}{\tau} + a)v(t_n + \tfrac{\tau}{2}, x_0 + \tfrac{h}{2}) \ . \end{aligned}\right\} \tag{13}$$

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

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

$$\left.\begin{aligned} v(t_n + \tfrac{\tau}{2}, x) &= v(t_n + \tfrac{\tau}{2}, x_0) + \tfrac{(x-x_0)}{h}W(m_0) \ , \\ W(m_0) &= \tfrac{u(m_+) - 2u(m_0) + u(m_-)}{h} \ . \end{aligned}\right\} \tag{14}$$

Then

$$v(t_n + \frac{\tau}{2}, x_0 \pm \frac{h}{2}) = v(t_n + \frac{\tau}{2}, x_0) \pm \frac{1}{2}W(m_0) \ . \tag{15}$$

Substitution of (15) into (13) and elimination of $v(t_n + \frac{\tau}{2}, x_0)$ yields the following explicit second order scheme for evaluating of $u(n_0)$ at the new layer

$$u(n_0) = \frac{1}{2}[(1+k)u(m_-) + (1-k)u(m_+) - (1-k^2)hW(m_0)] \ , \tag{16}$$

or

$$\delta u = \frac{1}{2}[(1+k)u(m_-) - 2u(m_0) + (1-k)u(m_+) - (1-k^2)hW(m_0)] \ . \tag{17}$$

As you could see in the scheme proposed above the supplementary variable is not used. Also it may be mentioned that scheme (16-17) in linear case is coincided with well-known Lax-Wendroff and MacCormick schemes written for the full step.

4. Applicatition to problems with discontinuous solutions

4.1. **Selection criterion for choosing of schemes.** Both schemes (9) and (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 will have high frequency spurious oscillations near the discontinuities. In [1-2] it was shown, that using a combination of schemes (9) and (12) instead of one scheme alone on the fixed stencil allows to obtain the monotone solution without high frequency spurious oscillations near the discontinuities. To provide a monotone solution, in these approach in each nodal point of the new layer two solutions by schemes (9) and (12) are evaluated and one of them is chosen according to a *special criterion*, as a final solution. The criterion proposed in the cited papers is based on the estimation of the average value of the differential operator of the governing equation in the cell of finite difference grid.

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

$$M_L(u) = \frac{\int_D L(u)dxdt}{\int_D dxdt} \ . \tag{18}$$

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

$$M_L(u) = \frac{\int_D (\frac{\partial u}{\partial t} + \frac{\partial(au)}{\partial x})dxdt}{\int_D dxdt} = \frac{\oint_{\partial D} (-udx + audt)}{\int_D dxdt} \ . \tag{19}$$

Let us choose D as an elementary cell of finite difference grid with vertexes m_0, m_+, n_+ and n_0 (see Fig.1). Then evaluating integrals in (12) over this region we obtain

$$\int_D dxdt = h\tau \ ,$$

$$\oint_{\partial D} (-udx + audt) = -\int_{m_0}^{m_+} udx + \int_{m_+}^{n_+} audt + \int_{n_0}^{n_+} udx - \int_{m_0}^{n_0} audt \ .$$

Integrals in right-hand side of the last formula are evaluated by the Euler-Gregory quadrature formula. Then we have

$$\int_{n_0}^{n_+} u dx = \tfrac{h}{2}(u_{n_0} + u_{n_+}) - \tfrac{h^2}{12}(v_{n_+} - v_{n_0}) + O(h^5) ,$$

$$\int_{m_0}^{m_+} u dx = \tfrac{h}{2}(u_{m_0} + u_{m_+}) - \tfrac{h^2}{12}(v_{m_+} - v_{m_0}) + O(h^5) ,$$

$$\int_{m_+}^{n_+} au dt = \tfrac{a\tau}{2}(u_{m_+} + u_{n_+}) - \tfrac{a\tau^2}{12}(w_{n_+} - w_{m_+}) + O(\tau^5) ,$$

$$\int_{m_0}^{n_0} au dt = \tfrac{a\tau}{2}(u_{m_0} + u_{n_0}) - \tfrac{a\tau^2}{12}(w_{n_0} - w_{m_0}) + O(\tau^5) .$$

Here $v = \frac{\partial u}{\partial x}$ and $w = \frac{\partial u}{\partial t}$.

Thus we obtain

$$M_L(m_0) = \tfrac{1}{2\tau}[(1+k)(u_{n_+} - u_{m_0}) - (1-k)(u_{m_+} - u_{n_0})] +$$
$$\tfrac{h}{12\tau}[v_{n_0} + v_{m_+} - v_{m_0} - v_{n_+}] +$$
$$\tfrac{k}{12}[w_{n_0} + w_{m_+} - w_{m_0} - w_{n_+}] + O(h_*^3) .$$

Here we denote $h_* \sim h \sim \tau$.

Supposing that equation (1) is valid and the function u is satisfied to this equation, we have $w = -av$ and then we obtain

$$M_L(m_0) = \tfrac{h}{2\tau}[\tfrac{(1+k)(u_{n_+} - u_{m_0}) - (1-k)(u_{m_+} - u_{n_0})}{h} + \tag{20}$$
$$\tfrac{1-k^2}{6}(v_{n_0} + v_{m_+} - v_{m_0} - v_{n_+})] + O(h_*^3) .$$

Now we could consider four cases of seaching functions computing in points n_0 and n_+ by schemes (9) or (12).

Case I: u_{n_0}, v_{n_0} and u_{n_+}, v_{n_+} are computed by the scheme (9). Then excluding u_{n_0}, v_{n_0}, u_{n_+} and v_{n_+} in (20) according to formulas (9) we obtain the following expression

$$M_L^I(m_0) = \tfrac{a}{6k}(2k-1)(1-k)(\tfrac{u_{m_-} - 2u_{m_0} + u_{m_+}}{h} + \tag{21}$$
$$\tfrac{1-k}{2}v_{m_-} + kv_{m_0} - \tfrac{1+k}{2}v_{m_+}) + O(h_*^2) .$$

Case II: u_{n_0}, v_{n_0} are computed by the scheme (9) and u_{n_+}, v_{n_+} are computed by the scheme (12). Then excluding in (20) u_{n_0}, v_{n_0} according to formulas (9) and u_{n_+} and v_{n_+} according to formulas (12) we obtain the following expression

$$M_L^{II}(m_0) = -M_L^I(m_0) + \frac{1+k}{1-2k}M_L^I(m_+) + O(h_*^2) . \tag{22}$$

Case III: u_{n_0}, v_{n_0} are computed by the scheme (12) and u_{n_+}, v_{n_+} are computed by the scheme (9). Then excluding in (20) u_{n_0}, v_{n_0} according to formulas (12) and u_{n_+} and v_{n_+} according to formulas (9) we obtain the following expression

$$M_L^{III}(m_0) = \frac{1+k}{1-2k}M_L^I(m_0) + O(h_*^2) . \tag{23}$$

Case IV: u_{n_0}, vn_0 and u_{n+}, v_{n+} are computed by the scheme (12). Then excluding in (20) u_{n_0}, v_{n_0} and u_{n+} and v_{n+} according to formulas (12), we obtain the following expression

$$M_L^{IV}(m_0) = \frac{1+k}{1-2k}[M_L^{II}(m_0) + M_L^{I}(m_+)] + O(h_*^2) \ . \tag{24}$$

If grid values of functions u and v in all m_j points of the data time layer $t = t_n$ adjust according to the following formulas

$$\left.\begin{aligned} \frac{\partial u}{\partial x} &= v_j + O(h_*^2) \ , \\ \frac{\partial^2 u}{\partial x^2} &= \frac{\partial v}{\partial x} + O(h_*) \ , \end{aligned}\right\} \tag{25}$$

then we have

$$M_L^{I}(m_j) = O(h_*^2), \ M_L^{II}(m_j) = O(h_*^2), \ M_L^{III}(m_j) = O(h_*^2) \ M_L^{IV}(m_j) = O(h_*^2).$$

Thus, if $u \in C^3(D)$, then the numerical solution computed by schemes (9) or (12) approximates the average value of the transport equation operator with the second order approximation error. But in case $u \notin C^3(D)$ and, if initial data don't satisfy to conditions (22), the same order of approximation error should be obtained only in two special cases: 1) if $k = 1$, this case is corresponded to the pure method of characteristics; 2) if $k = 0.5$ for the scheme (9).

In general case the "good" solution is corresponded to the "good" approximation of conditions (25) on all data layers. For the shock wave type solutions it is impossible to provide a good approximation of conditions (25), because, if initial data on any layer have points of discontinuities do not coincide with the grid points for all spatial grid steps $h- > 0$ and also, if these data are restricted, then the first term in round brackets in the formula (21) and the analogous terms in formulas (22-24) means

$$\left.\begin{aligned} H_L^{I}(m_0) &= \tfrac{a}{6k}(2k-1)(1-k)\left(\tfrac{(u_{m_-} - 2u_{m_0} + u_{m_+}}{h}\right) \ . \\ H_L^{II}(m_0) &= -H_L^{I}(m_0) + \tfrac{1+k}{1-2k} H_L^{I}(m_+) \ , \\ H_L^{III}(m_0) &= \tfrac{1+k}{1-2k} H_L^{I}(m_0) \ , \\ H_L^{IV}(m_0) &= \tfrac{1+k}{1-2k}[H_L^{II}(m_0) + H_L^{I}(m_+)] \ , \end{aligned}\right\} \tag{26}$$

are not restricted and the direct application of schemes (9) and (12) leads to the arising of spurious oscillations in numerical solutions in regions near the points of discontinuity.

In [1-2] basing on analysis of quantities H_L^i, $(i = I, II, III, IV)$ the pure high resolution algorithm was proposed. In this algorithm in all grid points at the first stage two solutions are computed by schemes (9) and (12). At the second stage the final solution is selected among two above mentioned solution according to the following criterion.

Let we have computed the solution at the new layer from the first point to the point n_0. Now our goal is to find a final solution at the point n_+. Let us consider the following finite difference evaluated at the previous time level $s(m_0) = u_{m_0+2} - u_{m_0}$.

Let at the point n_0 the final solution is corresponded to the solution obtained by scheme (9). Then, if $s(m_0) \le 0$, we choose as a final solution at the point n_+ such solution of (9) and (12) that is corresponded to the maximal value of quantities H_L^I and $H_L^I I$. If $s(m_0) > 0$, then we take as a final solution such solution of (9) and (12) that is corresponded to the minimal value of quantities H_L^I and $H_L^I I$.

Let at the point n_0 the final solution is corresponded to the solution obtained by scheme (12). Then, if $s(m_0) \leq 0$, we choose as a final solution at the point n_+ such solution of (9) and (12) that is corresponded to the maximal value of quantities $H_L^I II$ and $H_L^I V$. If $s(m_0) > 0$, then we take as a final solution such solution of (9) and (12) that is corresponded to the minimal value of quantities $H_L^I II$ and $H_L^I V$.

Results of computations presented in [1-2] shows that this algorithm allows to obtain high resolution monotone solutions in case when initial data have a complicated shock-wave structures.

4.2. **Hybrid Schemes.** Unfortunately criterion proposed above is very complicated and not suitable for parallel computations because it takes into account the history of computations at the new layer. Further we consider another way to construct a monotone solutions using hybrid algorithms. In this approach the first order monotone schemes are used instead of the high resolution schemes only in narrow regions where discontinuities of solutions arisen. In fact, most of the modern high resolution schemes [9-10] are of this type because they usually implicitly set restrictions on coefficients lowering the order of approximation in zones where discontinuities of solution could arise.

As shown in [3] for the quasi-characteristics scheme with the approximation of outward derivative at the middle layer, if we set $W(m_0) = 0$ in formulas (16-17), then we obtain a conservative scheme of the first order approximation. In [3] it was proposed to use this property to construct a hybrid modification of the quasi-characteristics scheme with the first order approximation only in narrow regions where in nonlinear case $(a = a(U))$ discontinuities of solutions should be arisen and with the second order approximation in all other regions. The switching was realized by the following manner. Let $W(m_+)$ and $W(m_-)$ are the second order differences defined analogously to $W(m_0)$ by the following formulas

$$W(m_-) = \frac{u(m_0) - 2u(m_-) + u(m_- - 1)}{h} ,$$

$$W(m_+) = \frac{u(m_+ + 1) - 2u(m_+) + u(m_0)}{h} .$$

Then, to compute the final value of $W(m_0)$, we shall use the following formulas

$$\left.\begin{array}{l} if\ W(m_+)W(m_-) > 0,\ then\ W(m_0) = \frac{U(m_+) - 2U(m_0) + U(m_-)}{h} ; \\ if\ W(m_+)W(m_-) \leq 0,\ then\ W(m_0) = 0 . \end{array}\right\} \qquad (27)$$

For the scheme with half-sum approximation of outward derivatives the anologous hybrid algorithm was proposed in [5]. According to this algorithm solution of considering problem is evaluated by formulas (12) in both cases $W(m_+)W(m_-) > 0$ and $W(m_+)W(m_-) \leq 0$, but in the last case the intial data at the data layer are modified as follows: $v(m_-) = v(m_+) = 0$. In the first case the appropriate initial data are taken without modification.

5. Conclusions.

Numerical solutions [1-8] of various nonlinear initial boundary value problems for hyperbolic equations computed by quasi-characteristics schemes considered above shows, that these schemes could be applied to solution of various hyperbolic problems with high accuracy. These schemes could be efficiently realized even on the personal computers and workstations, because taking into account the nature of hyperbolic equations they could deliver high precision solution on the rough meshes.

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