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# Application of the principle of minimizing the derivative to the construction of finite-difference schemes for computing discontinuous solutions of gas dynamics ☆

V.P. Kolgan (1940–1978)

Progress in computer technology now allows the application of numerical methods to some practical multidimensional steady and unsteady gas flows. While selecting a numerical method, preference should be given to higher-order schemes, since they allow the study of the fine features of the solution and the reduction of the computation time. In general, however, solutions of non-stationary nonlinear equations of gas dynamics are not smooth and may include strong discontinuities, such as shock waves or contact discontinuities. This fact is important for choosing an appropriate numerical scheme. If the strong discontinuities are extracted from the simulation domain and traced (shock fitting), while the rest of the flow is smooth, it is possible to use numerical schemes with approximation close to the second order [1–3]. However, if the number of discontinuities increases with time leading to a complicated pattern, the application of the shock-fitting approach becomes difficult. In this case it is preferable to apply shock-capturing schemes [4–6], which have a lower order of approximation but allow the integration of the governing equations through the discontinuities without extracting their surfaces. Shock-capturing schemes of a higher order of approximation are currently under development [7–9].

In this paper, certain aspects of constructing a numerical scheme applicable to discontinuous flows of gas dynamics are discussed using the idea of minimizing the derivatives of the solution. A numerical scheme that is second-order accurate in space and first-order accurate in time is developed for the model equation $u_t + u_x = 0$. The properties of this scheme are analyzed and the conditions for its stability and monotonicity are formulated. These results are then used in devising a similar scheme for the non-stationary one-dimensional equations of gas dynamics. The performance of the new scheme is compared to that of other schemes, using the break-up of an initial discontinuity (Riemann problem) as an example.

## 1

First, we discuss some general properties of different numerical schemes for the model equation

$$u_t + u_x = 0. \tag{1}$$

The general solution of this equation is

$$u = f(x - t), \tag{2}$$

where $f(x) = u(x,0)$ is the initial value of the function $u$ at $t = 0$. If the solution is sought on a finite interval, then some boundary condition has to be applied only at the left starting point of the interval, while the condition at the right end of the interval is determined by Eq. (1) itself.

While computing discontinuous solutions of gas dynamics, it is generally more convenient to solve the equations written as conservation laws, rather than in their differential form, which is applicable only to smooth solutions. Model Eq. (1) may also be cast into conservation form:

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$$\oint (u dx - u dt) = 0. \tag{3}$$

In most cases, the numerical solution of gas dynamic problems can be reduced to a certain procedure that is repeated for every time step. Below we outline this procedure in general terms. The simulation domain is split into computational cells where the mean values of mass, momentum, and energy are known at time $t = t_0$. We assume that the spatial grid is uniform with $\Delta x = h$, and $u_n$ denotes the values of the function $u$ in the centers of the computational cells which are at $x_n = nh$:

$$u_n = u(nh, t_0). \tag{4}$$

The coordinates of the cell boundaries are

$$x_{n+1/2} = (n + 1/2)h = \frac{1}{2}(x_n + x_{n+1}). \tag{5}$$

Next, some approximation of the solution is constructed between the cell centers. This approximation is used for subsequent calculation of the numerical solution after a time interval $\tau$ in the centers of the cells:

$$u^n = u(nh, t_0 + \tau). \tag{6}$$

The accuracy of this approximation determines the order of accuracy of the scheme. The flow parameters may be assumed to be constant [5], linear, parabolic, etc., functions of the coordinates inside the cells. There are also schemes [10] based on approximating the continuous flow with discrete moving particles.

Once the approximation type inside the cells is chosen, a model describing the transport of mass, momentum, and energy between the neighboring cells needs to be developed. Several such transport models consistent with the laws of gas dynamics are available, for example:

- fluxes through the cell boundaries are described by the motion of discrete particles with individual values of mass, momentum and energy;
- flow at the boundary is computed from a Taylor expansion in time; the time derivatives are expressed in terms of spatial derivatives, known from the chosen spatial approximation (in this case, smooth flow near the boundary is assumed);
- an arbitrary discontinuity at the boundary is allowed and the fluxes between the cells are computed from the solution of the corresponding Riemann problem.

The last two transport mechanisms can be considered as local solutions of the equations of gas-dynamics. The above models are used for time integration to determine the increments of the gas parameters in every cell after $\tau$. For the model equation, we have

$$\Delta_{n+1/2} = \int_{t_0}^{t_0+\tau} u(x_{n+1/2}, t) dt, \tag{7}$$

where $u(x_{n+1/2}, t)$ depends on the spatial approximation and the transport model; $\Delta_{n+1/2}$ is the flux of quantity $u$ between the cells $n$ and $n + 1$. In this manner, various numerical schemes can be obtained for the model equation from the corresponding conservation laws. For stability, some additional limitation should be imposed on the time step $\tau$.

It should be noted that any scheme with constant coefficients for Eq. (1), written as

$$u^n = \sum_{k=-N}^{k=N} a_k u_{n-k}, \quad \sum_{k=-N}^{k=N} a_k = 1, \quad a_k = \text{const.}, \tag{8}$$

may be also written as

$$u^n = u_n + F_{n-1/2} - F_{n+1/2}, \tag{9}$$

where functions $F_{n\pm1/2}$ describe the selected transport mechanism between cells $n$ and $n \pm 1$:

$$F_{n+1/2} = \sum_{k=1-N}^{N} c_k u_{n+k}. \tag{10}$$

It can be shown that if the coefficients $a_k$ are even,

$$a_k = a_{-k} \quad (k = 1, 2, \ldots, N), \tag{11}$$

then the coefficients $c_k$ are odd:

$$c_{1+i} + c_{-i} = 0 \quad (i = 0, 1, \ldots, N - 1). \tag{12}$$

Similarly, if the $a_k$ are odd,

$$a_k = -a_{-k} \quad (k = 1, 2, \ldots, N), \tag{13}$$

then the $c_k$ are even:

$$c_{i+1} = c_{-i} \quad (i = 0, 1, \ldots, N-1). \tag{14}$$

Indeed, from (8) and (9),

$$\sum_{k=-N}^{k=N} a_k u_{n+k} = u_n + \sum_{k=1-N}^{N} c_k u_{n+k-1} - \sum_{k=1-N}^{N} c_k u_{n+k} = u_n - \sum_{k=1-N}^{N} c_k u_{n+k} + \sum_{k=-N}^{N-1} c_{k+1} u_{n+k}. \tag{15}$$

Eq. (15) holds for an arbitrary choice of $u$, which means that the coefficients in front of any $u_i$ on either side of this equation should be equal.

Therefore,

$$\begin{aligned}
&a_{-N} = c_{1-N},\\
&a_{1-N} = -c_{1-N} + c_{2-N},\\
&\ldots\\
&a_{-1} = -c_{-1} + c_0,\\
&a_0 = 1 - c_0 + c_1,\\
&a_1 = -c_1 + c_2,\\
&\ldots\\
&a_{N-1} = -c_{N-1} + c_N,\\
&a_N = -c_N.
\end{aligned} \tag{16}$$

These relations give a one-to-one correspondence between the coefficients $a_k$ and $c_k$ and allow us to prove the odd-even relation between the coefficients $a_k$ and $c_k$. Indeed, for even $a_k$, from the first and last equations of (16) it follows that $c_{1+i} + c_{-i} = 0$ for $i = N-1$. Similarly, from the second and second-to-last equations of (16) the same relation follows for $i = N-2$, etc. In the same manner, it can be shown that if the $a_k$ are odd, the $c_k$ are even.

The simplicity of the exact solution (2) for model Eq. (1) ensures that the analysis of even the schemes that allow for an arbitrary discontinuity at the cell interfaces is quite tractable.

Assuming a piecewise constant approximation of the parameters inside every cell, and solving the Riemann problem at the boundaries, we get the following first-order scheme:

$$u^n = u_n + (u_{n-1} - u_n)\frac{\tau}{h}. \tag{17}$$

Thus, the flux function $F_{n+1/2}$, describing the transport processes between neighboring cells, is

$$F_{n+1/2} = u_n \frac{\tau}{h}. \tag{18}$$

This scheme for model Eq. (1) is analogous to Godunov's scheme for gas dynamics [5]. The scheme is stable for $\tau/h < 1$ and is optimal among the constant-coefficient schemes with a three-point stencil in the sense that it preserves monotonicity of the solution.

Similarly, using linear and quadratic interpolations inside the computational cells, one can construct first- and second-order schemes analogous to those of Lax and Lax–Wendroff.[1]

## 2

In the following, we assume linear interpolation for the function $u$ inside the cells. The gradient of $u$ is chosen using values of the function in the centers of the two neighboring cells. For example, inside cell $n$, that is, for $x_{n-1/2} < x < x_{n+1/2}$,

$$u(x) = u_n + k_n(x - x_n). \tag{19}$$

The gradient $k_n$ inside cell $n$ does not affect, up to $O(h^3)$ terms, the value of the spatial integral of $u$ which appears in the conservation law (3):

$$\int_{x_{n-1/2}}^{x_{n+1/2}} u dx = u_n h + O(h^3). \tag{20}$$

Therefore, while designing a second-order accurate scheme, $k_n$ may be computed in several different ways from the values of $u_{n-1}$, $u_n$, and $u_{n+1}$. In particular, $k_n$ can be defined by one-sided finite differences requiring the knowledge of $u$ in just two points:

[1] *Translator's note:* This statement is incorrect and immediately contradicted by what follows in Section 2. Linear subcell interpolation yields second-order spatial accuracy, quadratic interpolation will yield third-order accuracy. The Lax–Friedrichs scheme is only first-order and may be regarded as Godunov's scheme on a staggered grid. The Lax–Wendroff scheme may be obtained by linear subcell interpolation that is downwind biased; this is never done in practice.

$$(k_n)_{left} = \frac{\Delta_{n-1}}{h}, \quad (k_n)_{right} = \frac{\Delta_n}{h}, \tag{21}$$

where $\Delta_n = u_{n+1} - u_n$.

To minimize the gradient of $u$ inside the cell, the smaller in absolute value of these two possibilities is chosen:

$$k_n = \begin{cases} (k_n)_{right} & \text{if } |\Delta_n| < |\Delta_{n-1}|, \\ (k_n)_{left} & \text{otherwise}, \end{cases} \tag{22}$$

or, equivalently,

$$k_n h = \begin{cases} \Delta_n & \text{if } |\Delta_n| < |\Delta_{n-1}|, \\ \Delta_{n-1} & \text{otherwise}. \end{cases}$$

This approximation is based on one-sided differences and the suggestion to minimize the derivative, and it achieves a more accurate description of the parameters inside the computational cells in the presence of discontinuities. For smooth solutions, the approximation order is $O(h^2)$.

Let us now consider the discontinuities which may appear at the cell boundaries as a result of interpolation inside the cells. The solution of the problem of the discontinuity break-up at each interface provides the most accurate description of the transport processes between the cells. However, solving the Riemann problem for the nonlinear equations of gas dynamics with nonuniform parameters on either side of the discontinuity is extremely tedious. Therefore, for the proposed level of approximation, we will solve only the Riemann problem arising at the initial time, when the solution does not depend on the gradients on either side of the interface. In this case the problem is self-similar and can readily be solved. This approximation reduces the time-accuracy of the method to the first order; however, in time-marching to a steady state, when only the solution at $t \to \infty$ is sought, the order of accuracy in time is inconsequential.

For the model equation, applying this approach to formulating the Riemann problem is equivalent to assuming a constant value for the function $u$ which is equal to the left limit value at the discontinuity for $t = t_0$. The error of this approximation is $O(\tau)$.

Applying integral conservation laws in each cell for the time interval $\tau$ we get the following numerical scheme, consisting of four branches:

$$\begin{aligned}
&(1) \quad u^n = u_n + \frac{\tau}{2h}(u_{n-1} - u_{n+1}) = u_n - \frac{\tau}{2h}(\Delta_{n-1} + \Delta_n), \quad |\Delta_{n-2}| \geqslant |\Delta_{n-1}| \geqslant |\Delta_n|; \\
&(2) \quad u^n = u_n + \frac{\tau}{2h}(-u_{n-2} + 4u_{n-1} - 3u_n) = u_n + \frac{\tau}{2h}(\Delta_{n-2} - 3\Delta_{n-1}), \quad |\Delta_{n-2}| \leqslant |\Delta_{n-1}| \leqslant |\Delta_n|; \\
&(3) \quad u^n = u_n + \frac{\tau}{h}(u_{n-1} - u_n) = u_n - \frac{\tau}{2h}\Delta_{n-1}, \quad |\Delta_{n-2}| \geqslant |\Delta_{n-1}| \leqslant |\Delta_n|; \\
&(4) \quad u^n = u_n + \frac{\tau}{2h}(-u_{n-2} + 3u_{n-1} - u_n - u_{n+1}) = u_n + \frac{\tau}{2h}(\Delta_{n-2} - 2\Delta_{n-1} - \Delta_n), \quad |\Delta_{n-2}| \leqslant |\Delta_{n-1}| \geqslant |\Delta_n|.
\end{aligned} \tag{23}$$

This scheme uses a five-point stencil and has non-constant coefficients. The approximation error of this scheme for smooth solutions is

$$\varepsilon = O(h^2) + O(\tau),$$

i.e., the scheme is second-order accurate in space and first-order accurate in time.

## 3

Stability is one of the fundamental requirements for any practical numerical scheme. Another important requirement is preservation by the scheme of the qualitative behavior of the solution, e.g., monotonicity [5]. Now we turn our attention to these properties for scheme (23). Since the scheme has variable coefficients, the usual methods of analysis (Fourier expansion) are not applicable. However, we can construct the proof through a consideration of some inequalities.

First, we prove the following lemma for scheme (23):

$$\text{for} \quad \tau/h \leqslant 1/2, \quad \text{if} \quad \Delta_{n-1} \geqslant 0 \quad \text{then} \quad u_{n-1} \leqslant u^n \leqslant u_n, \quad \text{otherwise} \quad u_{n-1} \geqslant u^n \geqslant u_n.$$

We go through the proof for $\Delta_{n-1} \geqslant 0$ (the case $\Delta_{n-1} < 0$ can be handled in a similar manner).

If the first branch of scheme (23) is executed, then, on the one hand, we have

$$u^n - u_n = -\frac{\tau}{2h}(\Delta_{n-1} + \Delta_n) \leqslant 0 \quad \text{for} \quad |\Delta_{n-2}| \geqslant |\Delta_{n-1}| \geqslant |\Delta_n|.$$

However, by adding and subtracting $u_{n-1}$ from this equation, we can show that

$$u^n - u_{n-1} = \Delta_{n-1} - \frac{\tau}{2h}(\Delta_{n-1} + \Delta_n) \geqslant \left(1 - \frac{\tau}{h}\right)\Delta_{n-1} \geqslant 0.$$

The last of these inequalities holds for $\tau/h < 1$.

Next, we consider the second branch of scheme (23). Then

$$u^n - u_n = \frac{\tau}{2h}(\Delta_{n-2} - 3\Delta_{n-1}) \leqslant 0 \quad \text{for} \quad |\Delta_{n-2}| \leqslant |\Delta_{n-1}| \leqslant |\Delta_n|.$$

However, $u^n$ is also bounded from below:

$$u^n - u_{n-1} = \Delta_{n-1} + \frac{\tau}{2h}(\Delta_{n-2} - 3\Delta_{n-1}) \geqslant \left(1 - \frac{2\tau}{h}\right)\Delta_{n-1} \geqslant 0.$$

For the last inequality to hold here we have to assume that $\tau/h < 1/2$.

Now we investigate the third branch of the scheme:

$$u^n - u_n = -\frac{\tau}{h}\Delta_{n-1} \leqslant 0 \quad \text{for} \quad |\Delta_{n-2}| \geqslant |\Delta_{n-1}| \leqslant |\Delta_n|.$$

In this case we also have the condition

$$u^n - u_{n-1} = \left(1 - \frac{\tau}{h}\right)\Delta_{n-1} \geqslant 0,$$

which holds for $\tau/h \leqslant 1$.

Finally, we consider the last, fourth branch of (23):

$$u^n - u_n = \frac{\tau}{2h}(\Delta_{n-2} - 2\Delta_{n-1} - \Delta_n) \leqslant 0 \quad \text{for} \quad |\Delta_{n-2}| \leqslant |\Delta_{n-1}| \geqslant |\Delta_n|.$$

However, on the other hand,

$$u^n - u_{n-1} = \Delta_{n-1} + \frac{\tau}{2h}(\Delta_{n-2} - 2\Delta_{n-1} - \Delta_n) \geqslant \Delta_{n-1}\left(1 - 2\frac{\tau}{h}\right) \geqslant 0,$$

which holds for $\tau/h \leqslant 1/2$. Thus, the lemma is proved.

Now, using this lemma it is easy to prove the stability of the scheme.

We need to show that if $\max_n|u_n| < M$, then $\max_n|u^n| \leqslant \max_n|u_n| < M$. Indeed, using the lemma we have

$$|u^n| \leqslant \max(|u_{n-1}|, |u_n|) \leqslant \max_n |u_n|,$$

from which it follows that

$$\max_n(|u^n|) \leqslant \max_n |u_n| < M.$$

Now, we show that the scheme preserves the monotonicity of the function $u$ for $\tau/h < 1/2$. Assuming that $\Delta_n \geqslant 0$ for all $n$, from the lemma we have

$$u_{n-1} \leqslant u^n \leqslant u_n, \quad u_n \leqslant u^{n+1} \leqslant u_{n+1}$$

and, therefore, $u^n \leqslant u^{n+1}$.

Similarly, monotonicity can be proven for $\Delta_n \leqslant 0$ as well. A more involved analysis may be invoked to show that the scheme remains monotone for $\tau/h \leqslant 2/3$.

## 4

Now, we turn our attention to the nonlinear equations of ideal gas dynamics

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0,\\
&\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial x}(p + \rho u^2) = 0,\\
&\frac{\partial}{\partial t}\left(\frac{p}{\gamma - 1} + \frac{\rho u^2}{2}\right) + \frac{\partial}{\partial x}\left(u\left(\frac{\gamma p}{\gamma - 1} + \frac{\rho u^2}{2}\right)\right) = 0.
\end{aligned} \tag{24}$$

Here $p$ is pressure, $\rho$ is density, $u$ is speed, and $\gamma$ is the specific heats ratio.

Below, we construct a scheme similar to (23) for this set of equations. We assume a uniform grid with the quantities $p_n$, $\rho_n$, and $u_n$ defined at the centers of the computational cells. Inside the cells we use a linear interpolation, consistent with minimization of the derivative. This interpolation is used to evaluate the gas parameters at the cell boundaries.

Then, we use the solution of a Riemann problem with these parameters to get the initial values at $t = t_0 + 0$ for the fluxes of mass, momentum and energy between the cells.

Finally, applying the integral conservation laws we get a finite-difference scheme for computing new values $p^n$, $\rho^n$ and $u^n$ at time $t = t_0 + \tau$:

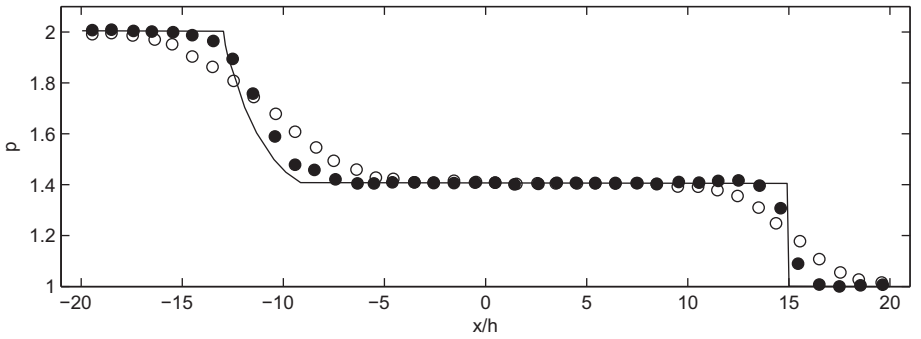


**Fig. 1.** Pressure distribution along the coordinate. Solid line – exact solution, solid circles – the numerical method described in this paper, open circles – Godunov's method for Euler coordinates [11].

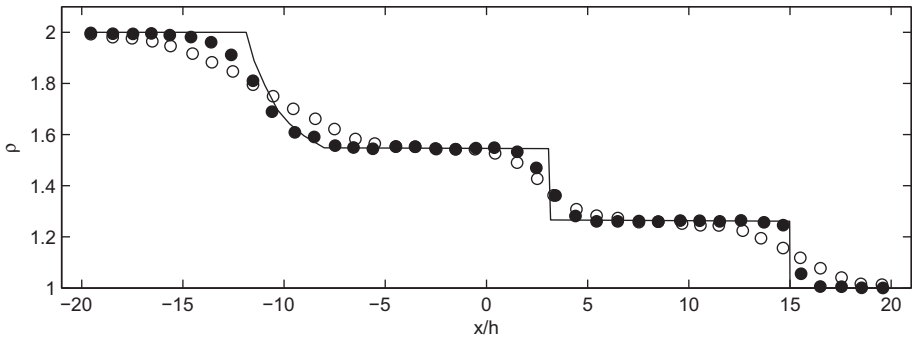


**Fig. 2.** Density distribution along the coordinate. Solid line – exact solution, solid circles – the numerical method described in this paper, open circles – Godunov's method for Euler coordinates [11].

$$
\begin{aligned}
&\rho^n = \rho_n + \frac{\tau}{h}((RU)_{n-1/2} - (RU)_{n+1/2}),\\
&(\rho u)^n = (\rho u)_n + \frac{\tau}{h}((P + RU^2)_{n-1/2} - (P + RU^2)_{n+1/2}),\\
&\left(\frac{p}{\gamma-1} + \frac{\rho u^2}{2}\right)^n = \left(\frac{p}{\gamma-1} + \frac{\rho u^2}{2}\right)_n + \frac{\tau}{h}\left\{\left(U\left(\frac{\gamma P}{\gamma-1} + \frac{RU^2}{2}\right)\right)_{n-1/2} - \left(U\left(\frac{\gamma P}{\gamma-1} + \frac{RU^2}{2}\right)\right)_{n+1/2}\right\}.
\end{aligned}
\tag{25}
$$

Here, $P$, $R$, and $U$ correspond to pressure, density, and speed at the cell boundaries at $t = t_0 + 0$. Obviously, scheme (25) is second-order accurate in space and first-order accurate in time. It may be expected, that this scheme is stable for

$$
\tau/h \leqslant \frac{1}{2|c|}, \tag{26}
$$

where $c$ is the maximum speed of propagation of disturbances appearing as a result of the break-up of the initial discontinuities. Condition (26) is formulated by analogy to the stability condition for the model equation. Physically, this condition means that the disturbances generated at the cell boundaries should not reach the center of the cell during one time step. Numerical experiments show that condition (26) in fact ensures the stability of calculations.

As an example, we show the results a solution of the Riemann problem with these initial conditions at $t = 0$:

$$
\left.\begin{array}{llllll}
\text{for} & x < 0, & p = 2, & \rho = 2, & u = 0,\\
\text{for} & x > 0, & p = 1, & \rho = 1, & u = 0.
\end{array}\right\}
\tag{27}
$$

For $t > 0$ three waves form as a result of the break-up of this discontinuity. These are: a rarefaction wave, propagating to the left through the denser gas, a contact discontinuity moving to the right and separating the denser gas from the less dense one, and a shock wave, also moving to the right. The results of the calculations are shown in Figs. 1 and 2.[2]

Scheme (25) gives a more accurate description of the flow parameters near the discontinuities then the original Godunov scheme. The results shown in the figures correspond to 37 time steps. For a larger number of time steps, the qualitative properties of the solution do not change.

[2] *Translator's note*: The data from the original figures have been digitized and re-plotted.

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