# A Method to Construct a Completely Conservative Lagrangian Difference Scheme for Gas Dynamics

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*A completely conservative Lagrangian difference scheme has been constructed for planar problems of gas dynamics. Difference operators $GRAD$ and $DIV$ have a simple and convenient form. Artificial viscosity is introduced along two directions of the scheme, therefore, even if strongly elongated cells are used a shock wave is "smeared" over the same number of cells regardless of the shock direction. From monotonicity of solution in 1D case, viscosity is derived as some non-linear combination of linear and quadratic viscosity. Results of numerical simulations are presented. For all 2D problems related to gas expansion in vacuum the simulation results obtained with the completely conservative scheme are more accurate than those obtained with the divergent and non-divergent schemes.*

## Introduction

Code MAX [1] implements both divergent and non-divergent schemes with respect to total energy, which are used during the Lagrangian step.
In a planar case the conservative Lagrangian scheme in the MAX code is the same as that proposed by C.Hirt and A.Amsden in Ref.[2] except for artificial viscosity. If kinetic energy is much higher than the internal one, even a minor relative error in calculated velocity might lead to significant errors in determined internal energy, which would show up through non-monotonicity of the numerical solution and negative internal energy in some cells. The non-divergent scheme, if applied in such cases, gives better results, but leads to imbalance of total energy. It is possible to try to eliminate the drawbacks of these two schemes by using a completely conservative difference scheme. Here "completely conservative" means that to construct the scheme, difference analogues of the basic laws of conservation (mass, momentum and total energy) are implemented in the same way as for the conservative scheme, and a difference analogue of the energy equation is written in the non-divergent form. The paper presents such a scheme. It approximates differential equation of internal energy and includes difference analogues of operators $div$ and $grad$ based on the law of conservation of total energy.

## 2D completely conservative Lagrangian difference scheme for gas dynamics

Integral laws of conservation for some volume $\omega$ moving with the material particles can be written as:

$$\frac{d}{dt}\iint_{\omega(t)} \rho d\omega = 0, \tag{1}$$

$$\frac{d}{dt}\iint_{\omega(t)} \rho \bar{W} d\omega = -\oint_{\gamma(t)} p\bar{n} d\gamma, \tag{2}$$

$$\frac{d}{dt}\iint_{\omega(t)} \rho\left(\frac{1}{2}\left|\bar{W}\right|^2 + \varepsilon\right) d\omega = -\oint_{\gamma(t)} p\left(\bar{n},\bar{W}\right) d\gamma, \tag{3}$$

where $\rho$ is density, $\bar{W}$ is a velocity vector, $p$ is pressure, $\varepsilon$ is specific internal energy. It is necessary to derive solution to the system of equations (1)-(3) in some domain $\Omega$ at specified initial and boundary conditions. In the planar case, let $\omega(t)$ be treated as area and $\gamma(t)$ as a contour limiting $\omega(t)$.

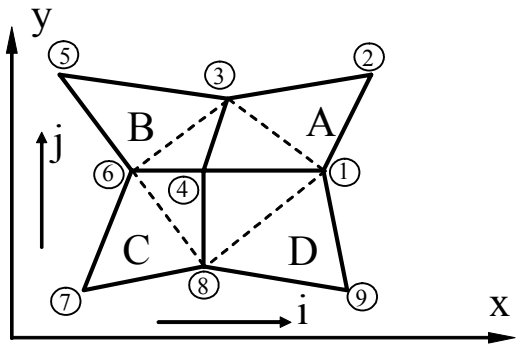


Fig. 1 Fragment of a difference mesh.

Domain $\Omega$ is covered with a quadrilateral mesh that can be mapped into a rectangular mesh in a square with some non-degenerate transformation. The quadrilaterals are called cells and their vertices are called nodes. Consider four adjacent cells. The nodes are labeled with digits as shown in Fig. 1 and cells are marked with letters A, B, C, and D.

The cell area is calculated with the following formula

$$S_A = \frac{1}{2}\left[(x_1 - x_3)(y_2 - y_4) + (y_1 - y_3)(x_4 - x_2)\right], \tag{4}$$

where $(x_\alpha, y_\alpha)$ are Cartesian coordinates of node $\alpha$ $(\alpha = 1,2,3,4)$.

Density $\rho$, energy $\varepsilon$, and pressure $p$ are referred to the cells and velocity $\bar{W} = [u, v]$ is referred to the nodes.

Define the cell mass as

$$M_A = \rho_A S_A .$$

Then the node mass is

$$M_4 = \frac{1}{4}(M_A + M_B + M_C + M_D).$$

Equation (1) means that cell masses are constant in time. The numerical method implemented in MAX complex [1] approximates equation (2) in the following way:

$$\frac{\bar{W}_4^{n+1} - \bar{W}_4^n}{\tau} + GRAD_4 p^{(\sigma)} = 0 \tag{5}$$

$$GRAD_4 p^{(\sigma)} =$$

$$\frac{1}{2M_4}\left( p_A^{(\sigma)}\begin{bmatrix} y_3-y_1 \\ x_1-x_3 \end{bmatrix} + p_B^{(\sigma)}\begin{bmatrix} y_6-y_3 \\ x_3-x_6 \end{bmatrix} + p_C^{(\sigma)}\begin{bmatrix} y_8-y_6 \\ x_6-x_8 \end{bmatrix} + p_D^{(\sigma)}\begin{bmatrix} y_1-y_8 \\ x_8-x_1 \end{bmatrix}\right) \quad (6)$$

$p_A^{(\sigma)} = \sigma p_A^{n+1} + (1-\sigma) p_A^n$ (in MAX scheme $\sigma = 1$).

Difference operator $GRAD$ (6) is used in numerical methods to approximate equation of motion pretty often, for example, in scheme D [3], in Wilkins method [4], etc.

Consider an equation of energy in the non-divergent form:

$$\rho \frac{d\varepsilon}{dt} + p \cdot div \bar{W} = 0 \quad .$$

Approximate it:

$$\frac{\varepsilon_A^{n+1} - \varepsilon_A^n}{\tau} + p_A^{(\sigma)} DIV_A \bar{W}^{(0.5)} = 0 , \quad (7)$$

where $\bar{W}^{(0.5)} = \dfrac{\bar{W}^{n+1} + \bar{W}^n}{2}$.

Derive $DIV_A \bar{W}^{(0.5)}$ for the law of conservation of total energy for the whole domain $\Omega$ (difference analogue of integral equation (3)).

Assume that $K_\Omega$ is a set of the mesh nodes, $N_\Omega$ is a set of cells, and $L_\Gamma$ is a set of boundary sections of the mesh.

Calculate a scalar product of equation (5) by vector $\bar{W}_4^{(0.5)} M_4$, sum over all mesh nodes and add the result to equation (7) multiplied by the cell mass and summed over all cells and obtain

$$\frac{\left[ \sum_{\alpha \in K_\Omega} M_\alpha \frac{\left|\bar{W}_\alpha^{n+1}\right|^2}{2} + \sum_{A \in N_\Omega} M_A \varepsilon_A^{n+1} \right] - \left[ \sum_{\alpha \in K_\Omega} M_\alpha \frac{\left|\bar{W}_\alpha^{n}\right|^2}{2} + \sum_{A \in N_\Omega} M_A \varepsilon_A^{n} \right]}{\tau} =$$

$$-\left( \sum_{\alpha \in K_\Omega} M_\alpha (\bar{W}_\alpha^{(0.5)}, GRAD_\alpha p^{(\sigma)}) + \sum_{A \in N_\Omega} M_A p_A^{(\sigma)} DIV_A \bar{W}^{(0.5)} \right).$$

To meet difference analogue (3), write down the condition:

$$\sum_{\alpha \in K_\Omega} M_\alpha (\bar{W}_\alpha^{(0.5)}, GRAD_\alpha p^{(\sigma)}) + \sum_{A \in N_\Omega} M_A p_A^{(\sigma)} DIV_A \bar{W}^{(0.5)} =$$

$$\sum_{\beta \in L_\Gamma} p_\beta (\bar{n}, \bar{W}^{(0.5)})_\beta \Delta l_\beta , \quad (8)$$

here $\Delta l_\beta$ is a length of boundary section $\beta$.

Operators $GRAD$ and $DIV$ meeting condition (8) are called *consistent* [**5**].

Condition (8) allows unique determination of the velocity divergence:

$$DIV_A \bar{W} = \frac{DUV_A}{M_A} ,$$

где $DUV_A = DH_A - DF_A + DR_A - DL_A$, (9)

$$DH_A = \frac{1}{2}\left[ (u_2+u_3)(y_3-y_2) + (v_2+v_3)(x_2-x_3) \right], \quad (10)$$

$$DR_A = \frac{1}{2}\left[ (u_1+u_2)(y_2-y_1) + (v_1+v_2)(x_1-x_2) \right], \quad (11)$$

$$DF_A = \frac{1}{2}\left[ (u_1+u_4)(y_4-y_1) + (v_1+v_4)(x_1-x_4) \right], \quad (12)$$

$$DL_A=\frac{1}{2}\left[(u_3+u_4)(y_3-y_4)+(v_3+v_4)(x_4-x_3)\right]. \qquad (13)$$

So, the system of equations (6) and (7) is completely determined. Expression for $DIV_A\bar{W}$ (10)-(13) is a natural and widely used approximation of the velocity vector flow through the boundary of cell $A$. The obtained difference scheme coincides with one of the versions of scheme proposed in Ref. [6], and it is an approximation of the second order with respect to spatial variables on the uniform mesh and of the first order with respect to time, though at σ=0.5 energy and motion equations are approximated to the second-order with respect to time.

To calculate flows with shock waves, it is necessary to introduce artificial viscosity in the difference scheme. In 1D case, this is done by introducing some addition to pressure. In 2D case two viscosities are introduced in [1]: viscosity in direction $j$ denoted as $QJ$, and one in direction $i$ - $QI$ (see Fig. 1). Formulas below are associated with viscosity in the $j$-direction, they are similar for the other direction. To include artificial viscosity in the equation of motion in [1], it is necessary to define:

$$GRADJ_4QJ=$$
$$-\frac{1}{2M_4}\begin{pmatrix} QJ_A(y_{12}-y_{34})+QJ_B(y_{34}-y_{56})+QJ_C(y_{67}-y_{48})+QJ_D(y_{48}-y_{19}) \\ QJ_A(x_{34}-x_{12})+QJ_B(x_{56}-x_{34})+QJ_C(x_{48}-x_{67})+QJ_D(x_{19}-x_{48}) \end{pmatrix},$$

here the following notations are used

$$x_{\alpha\beta}=\frac{x_\alpha+x_\beta}{2}, \quad y_{\alpha\beta}=\frac{y_\alpha+y_\beta}{2}.$$

Then rewrite the equation of motion in the following form:

$$\frac{\bar{W}_4^{n+1}-\bar{W}_4^n}{\tau}+GRAD_4p^{(\sigma)}+GRADJ_4QJ+GRADI_4QI=0. \qquad (14)$$

The equation of energy is:

$$\frac{\varepsilon_A^{n+1}-\varepsilon_A^n}{\tau}+p^{(\sigma)}DIV_A\bar{W}^{(0.5)}+QJ\cdot DIVJ_A\bar{W}^{(0.5)}+QI\cdot DIVI_A\bar{W}^{(0.5)}=0,$$

where

$$DIVJ_A\bar{W}^{(0.5)}=\frac{1}{2M_A}\Big((y_{12}-y_{34})\big(u_4^{(0.5)}+u_1^{(0.5)}-u_2^{(0.5)}-u_3^{(0.5)}\big)+$$
$$+(x_{34}-x_{12})\big(v_4^{(0.5)}+v_1^{(0.5)}-v_2^{(0.5)}-v_3^{(0.5)}\big)\Big),$$

Coordinates of the mesh nodes in all constructed difference operators are from the n-th time layer.

The latest operator was obtained from condition:

$$\sum_\alpha M_\alpha\bar{W}_\alpha^{(0.5)}GRADJ_\alpha QJ=-\sum_A M_AQJ_ADIVJ_A\bar{W}^{(0.5)},$$

which results for the law of conservation of total energy and is obtained similarly to (8).

What still remains to be done is way of determining $QJ$ and $QI$. Below we determine the form and viscosity coefficient for the 1D case and generalize them for the 2D case.

## Artificial viscosity

Write down a difference scheme approximating gas dynamic equations in 1D planar case including artificial viscosity. For short, use notations of Samarsky A.A:

$$u_i^{n+1}=\hat{u},\ u_i^n=u,\ p_{i+1/2}^{n+1}=\hat{p},\ p_{i+1/2}^n=p,\ q_{i+1/2}=q,$$

$$\hat{u}=u+\frac{\tau}{m}(p_{i-1}^{(\sigma)}-p^{(\sigma)})+\frac{\tau}{m}(q_{i-1}-q), \tag{15}$$

$$q=\begin{cases}\frac{\lambda}{m}(u-u_{i+1}), & если\, u-u_{i+1}>0\\ 0, & если\, u-u_{i+1}\le 0\end{cases} \tag{16}$$

$$\hat{\rho}=\frac{m}{\hat{V}}, \tag{17}$$

$$\hat{V}=V+\tau(\hat{u}_{i+1}-\hat{u}), \qquad V=x_{i+1}-x, \tag{18}$$

$$\hat{\varepsilon}=\varepsilon+\tau\frac{p^{(\sigma)}+q}{m}\left(u^{(0.5)}-u_{i+1}^{(0.5)}\right). \tag{19}$$

The reasoning below is done for a specific case for consistent two-term equation of state

$$p=(\gamma-1)\varepsilon\rho+c_0^2(\rho-\rho_0), \tag{20}$$

$$c^2=\frac{\gamma p}{\rho}+\frac{c_0^2\rho_0}{\rho},$$

c is adiabatic speed of sound.

Mass step is assumed constant. As in Ref. [1], derive $\lambda$ from the monotonicity of the difference solution for stationary shock wave.

Instead of scheme (15)-(19), consider scheme differing by $O(\tau^2)$

$$\hat{u}=u+\frac{\tau}{m}(p_{i-1}^{(\sigma)}-p^{(\sigma)})+\lambda_{i-1}\frac{\tau}{m^2}(u_{i-1}-u)-\lambda\frac{\tau}{m^2}(u-u_{i+1}), \tag{21}$$

$$\begin{aligned}\hat{p}=p+\frac{\tau}{2m}\rho^2\left[(c^2+a^2)(\hat{u}-\hat{u}_{i+1})+(c^2-a^2)(u-u_{i+1})\right]+\\ (1+\sigma(\gamma-1))\frac{\tau^2\rho^3c^2}{m^2}(u-u_{i+1})^2+(\gamma-1)\frac{\tau}{m^2}\rho\lambda(u-u_{i+1})^2.\end{aligned} \tag{22}$$

Substituting (22) in (21), obtain a three-point equation of $\hat{u}$, from which $\lambda$ can be derived.

Assume that at time $t=t^n$ a stationary shock wave is set.

$c_1^0,u_1^0,\rho_1^0,p_1^0$ and $c_2^0,u_2^0,\rho_2^0,p_2^0$ are values behind and in front of the front, respectively.

Gas dynamic values at the discontinuity meet the Hugoniot conditions.

Using an expression following from the Hugoniot relations in a specific case of EOS (20)

$$p_1^0-p_2^0=\rho_2^0(u_1^0-u_2^0)\left(\sqrt{c_2^2+\left(\frac{\gamma+1}{4}\right)^2(u_1^0-u_2^0)^2}+\frac{\gamma+1}{4}(u_1^0-u_2^0)\right),$$

and keeping monotonicity of the numerical profile of the velocity, obtain the following form of viscosity in 1D case

$$q=\begin{cases}\rho\Delta u\left(\sqrt{c^2+\left(\frac{\gamma+1}{4}\right)^2\Delta u^2}+\frac{\gamma+1}{4}\Delta u\right)\frac{\sqrt{4\chi^2+1}+1-2\chi}{2}, & если\, \Delta u>0\\ 0, & если\, \Delta u\le 0,\end{cases} \tag{23}$$

where $\chi^2=\sigma\left(\frac{\tau}{m}\rho c\right)^2$.

To simulate shock waves, difference methods employ mostly linear or quadratic viscosity or a combination of these two. The viscosity derived also has a form of some non-linear combination of those two viscosities: linear and quadratic. This viscosity differs by a factor from that proposed by V.F.Kuropatenko [**7**]. At $\sigma$=1 viscosity (23) absolutely coincides with the viscosity used in divergent and non-divergent MAX schemes.

Monotonicity of the difference solution to velocity puts a restraint on the time step

$$\tau\le\frac{2\sqrt{2}h_2c_2}{(\gamma+1)\Delta u^0\sqrt{\sigma}\sqrt{a_2^2+c_2^2}},$$

and monotonicity of density requires:

$$\tau\le\frac{h_2}{2\left(\sqrt{c_2^2+\left(\frac{\gamma+1}{4}\Delta u^0\right)^2}+\frac{\gamma+1}{4}\Delta u^0\right)-\sqrt{\frac{c_2^2+a_2^2}{2}}\sqrt{\sigma}},$$

$$\tau\le\frac{\sqrt{2}h_2}{\sqrt{a_2^2+c_2^2}\sqrt{\sigma}}.$$

In many 2D techniques artificial viscosity is introduces as an addition to pressure. It is defined similarly to 1D case, but in 2D case the role of $\Delta u$ is played by $-h\cdot div\bar{W}$, where $h$ is a typical cell size. When strongly elongated mesh cells are used in order to “smear” a shock wave over the same number of cells regardless of the shock motion direction, parameter $h$ has to be define as a cell size in direction of maximum compression and for this purpose difference tensor of strain rate is used. The MAX technique [1] solves this problem in another way. Direction-dependent viscosities are introduced in a cell, each counteracting the cell compression along the specific direction. From (23) viscosities $QI$ and $QJ$ are defined in the following way.

Denote

$$HI_A=\sqrt{(x_R-x_L)^2+(y_R-y_L)^2},\ HJ_A=\sqrt{(x_H-x_F)^2+(y_H-y_F)^2},$$

$$H_{\max_A}=\max(HI_A,HJ_A),\ \chi_A=\left(\frac{H_{\max}}{S}\right)_A\tau c_A\sqrt{\sigma},$$

$$K_A=\frac{\sqrt{1+4\chi_A^2}+1-2\chi_A}{2},$$

$$DJ_A=\max\{(DH_A-DF_A),DUV_A\},$$

$DUV$, $DH$, $DF$, $DR$, $DL$ are determined from formulas (9)-(13).

$$\Delta uJ_A=\begin{cases}-DJ_A/HI_A, & если DJ_A<0,\\ 0, & если DJ_A\ge 0,\end{cases}$$

$$QJ=\Delta uJ_A\rho_A\left(\frac{\gamma+1}{4}\Delta uJ_A+\sqrt{\left(\frac{\gamma+1}{4}\right)^2\Delta uJ_A^2+c_A^2}\right)K_A,$$

## Implementation of implicit difference scheme

At the next time step, gas dynamic values are calculated in two steps: explicit and iteration [1]. At the explicit step we determine preliminary velocity values for all mesh nodes by using formula (14) at $\sigma=0$:

$$\tilde{\bar{W}}_\alpha=\bar{W}_\alpha^n-\tau(GRAD_\alpha p+GRADJ_\alpha QJ+GRADI_\alpha QI)$$

As the zeroth approximation for the iteration process, select

$$\bar{W}^0=\tilde{\bar{W}},p^0=p^n.$$

Assume $\bar{W}^\nu,p^\nu$ are known, calculation of the values at the nest iteration cycle $\nu+1$ is done according to the following procedure:

1. $\bar{r}_\alpha^\nu=\bar{r}_\alpha^n+\tau\bar{W}_\alpha^\nu$;
2. determine $S_A^\nu$ (4) from the obtained $\bar{r}_\alpha^\nu$;
3. $\rho_A^\nu=\dfrac{M_A}{S_A^\nu}$;
4. $\varepsilon_A^\nu=\varepsilon_A^n-\tau(p_A^{(\sigma)}DIV_A\bar{W}^{(0.5)}+QJ\cdot DIVJ_A\bar{W}^{(0.5)}+QI\cdot DIVI_A\bar{W}^{(0.5)})$,

   where $p_A^{(\sigma)}=\sigma p_A^\upsilon+(1-\sigma)p_A^n$, $\bar{W}^{(0.5)}=\dfrac{\bar{W}^\upsilon+\bar{W}^n}{2}$;
5. $\delta p_A^{\nu+1}=\dfrac{f(\rho_A^\nu,\varepsilon_A^\nu)-p_A^\nu}{1+2(\kappa_A^\nu)^2}$, $\kappa_A^\nu=\dfrac{\tau c_A^\nu H_{\max_A}}{S_A}\sqrt{\sigma}$,

   $p=f(\rho,\varepsilon)$ is equation of state, c is adiabatic speed of sound;
6. $p_A^{\nu+1}=p_A^\nu+\delta p_A^{\nu+1}$;
7. $\bar{W}_\alpha^{\nu+1}=\bar{W}_\alpha^\nu-\tau\cdot\sigma\cdot GRAD_\alpha\delta p^{\nu+1}$,

$\alpha-$ runs through all mesh nodes, $A$ covers all mesh cells.

The iteration process stops when at some $\nu=\nu_k$ the following is valid

$$\frac{|\delta p^{\nu_k+1}|}{p_{\max}}<\varepsilon_0,$$

where $p_{\max}$ is maximum pressure at the *n*-th step.

Final values at the *n*+1-th step are determined by the formulas:

$$p_A^{n+1}=p_A^{\nu_k+1},\bar{W}_\alpha^{n+1}=\bar{W}_\alpha^{\nu_k+1},\ \bar{r}_\alpha^{n+1}=\bar{r}_\alpha^n+\tau\bar{W}_\alpha^{n+1},$$

$S_A^{n+1}$ is calculated from $\bar{r}_\alpha^{n+1}$, $\rho_A^{n+1}=\dfrac{M_A}{S_A^{n+1}}$,

$$\varepsilon_A^{n+1}=\varepsilon_A^n-\tau(p_A^{(\sigma)}DIV_A\bar{W}^{(0.5)}+QJ\cdot DIVJ_A\bar{W}^{(0.5)}+QI\cdot DIVI_A\bar{W}^{(0.5)}).$$

Below is one of simulations of the model problem on expansion of a triangular cylinder. The results obtained with the MAX code are compared to the analytical solutions.

## Expansion of a triangular cylinder

Based on paper by Suchkov V.A. [8], it is possible to construct an exact solution to the problem on a planar 2D expansion of a cylinder filled with ideal gas with $\gamma=2$, $\rho=1$, and $\varepsilon=0.5$. Cylinder cross-section with the $oxy$ plane orthogonal to the cylinder axis is a regular triangle with the side $b=1$. This solution is valid till rarefaction waves of all three planes converge at the cylinder center. At this moment gas boundary in the $oxy$ plane is a regular hexagon.

**Fig. 2** shows density fields obtained in calculations using non-divergent, divergent schemes of MAX technique and completely conservative scheme in comparison with the exact solution at time $t=0.289$. All solutions almost coincide at that time moment.

Calculations are continued till $t=1$. To compare the results obtained with different schemes, an approximate solution obtained in the following way is taken as a reference. At the latest time $t=0.289$ when the analytical solution still exists, its precise geometry is specified and covered with a fine uniform mesh and projection of the exact solution on this mesh is treated as initial distribution. Then calculation is done till $t=1$.

**Fig. 3** compares the results calculated with the non-divergent, divergent MAX schemes and the completely conservative scheme to the approximate solution. Calculation done with the completely conservative scheme is close to that obtained with the non-divergent scheme. This is explained by the fact that mesh in the center is very fine and time step in the calculations is very small. Solution obtained with the divergent scheme is non-monotonous. Numerical solution obtained with the completely conservative scheme appears to be the closest to the exact and approximate solutions.

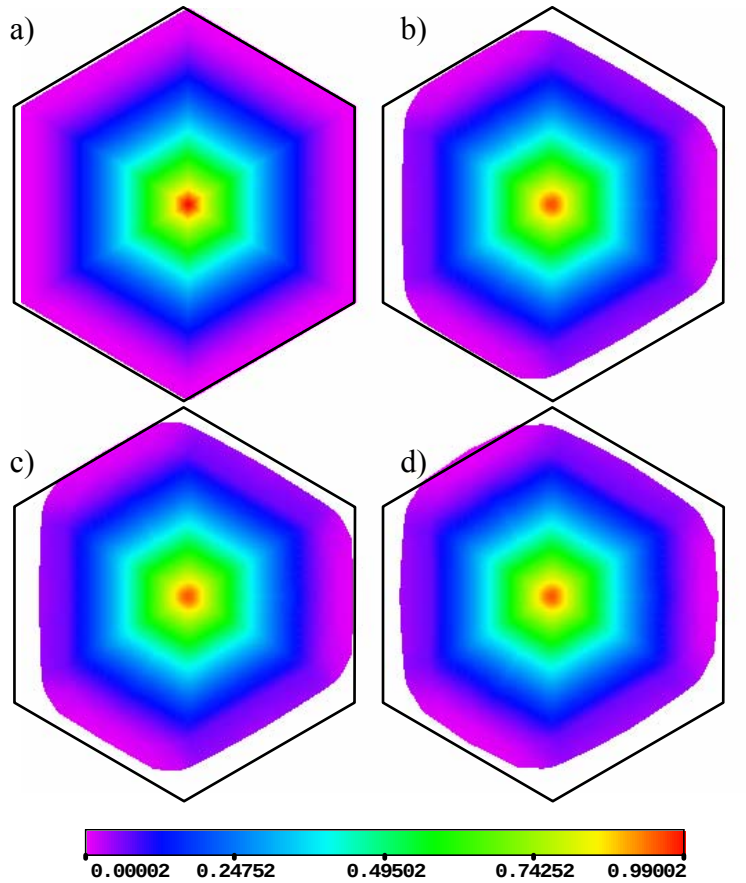


Fig. 2 Density field at time $t=0.289$,
a) – exact solution,
b) – non-divergent MAX scheme,
c) – completely conservative scheme,
d) – divergent MAX scheme.

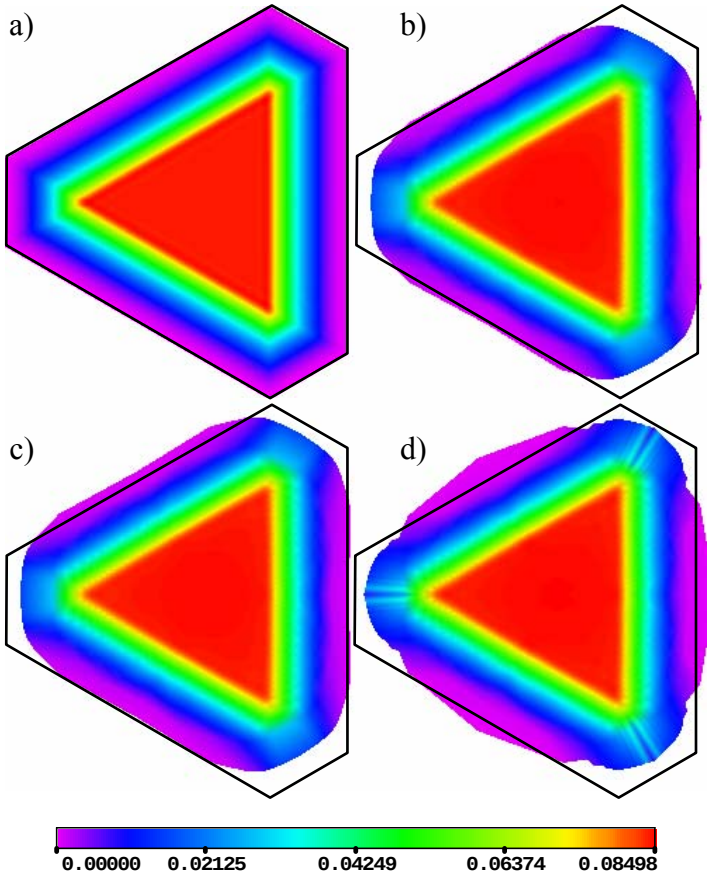


Fig. 3 Density field at time $t=1$,
a) – approximate solution,
b) – non-divergent MAX scheme,
c) – completely conservative scheme,
d) – divergent MAX scheme.

## Conclusion

The paper describes the constructed 2D completely conservative difference scheme for solving gas dynamic equations in Lagrangian variables for the planar case and artificial viscosity derived for this scheme. Based on the analysis of the results of numerical calculations obtained with the divergent and non-divergent MAX scheme and completely conservative scheme for a number of test problems having the exact solution, the following conclusions can be drawn:

- artificial viscosity similar to that in the MAX scheme, if used in the shock wave simulation, facilitates monotonicity of the value profiles, and in this case front of an infinitely strong shock is smeared over 4-5 computational intervals;
- for all 2D problems related to the gas expansion in vacuum the simulation results obtained with the completely conservative scheme are more accurate than those obtained with the divergent and non-divergent MAX schemes.

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