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On Conservative and Dissipative Difference Scheme of Dynamics of an Ideal Perfect Gas

F.B. Imranov*, A.G. Sokolov

Abstract. To approximate the continuity equation, a conservative difference scheme with a non-negative solution is considered. The energy equation is reduced to an analog of the continuity equation, the approximation of which ensures the non-negativity of the solution. For an ideal perfect gas, a grid analog of the energy inequality is obtained for a nonlinear implicit difference scheme.

Key Words and Phrases: approximation, conservatism of the grid analogue of the continuity equation, non-negativity of the grid density and energy, fully implicit nonlinear scheme, estimation of the grid energy.

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1. Introduction

The theoretical substantiation of the existence of generalized solutions of compressible continuous medium models was made in [5]. There, significant results were obtained for the barotropic gas model and the shallow water model close to it, as well as for the ideal perfect gas model. In [1], the results on the construction and study of a difference scheme for an inviscid barotropic gas are presented. In [4], we applied our difference schemes to calculate large-scale sea currents using the shallow water model. The results obtained in [1, 4] are transferred in this work to the case of the gas dynamics model of an inviscid ideal perfect gas, including the energy equation. The difference scheme is constructed under the assumption of differentiability of the solution of the original problem, while the energy equation is reduced to an equation completely analogous to the continuity equation.

*Corresponding author.

2. System of equations

The initial boundary value problem (system of Euler equations [2]) is considered for $t > 0, x \in \Omega$:

$$\begin{gathered} \frac{\partial \rho}{\partial t} + \mathrm{div} \rho \mathbf{u} = 0, \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \mathrm{grad}\, p = 0, \\ \frac{\partial e}{\partial t} + \mathrm{div}[(e+p)\mathbf{u}] = 0, \\ p = (\gamma - 1)\rho\varepsilon. \end{gathered} \tag{1}$$

Here ρ is the gas density, $\mathbf{u}$ is the velocity, p is the pressure, $\gamma = \mathrm{const} > 1$ is the given adiabatic index, ε is the specific internal energy, $e = \rho\varepsilon + \frac{1}{2}\rho\mathbf{u}^2$ is the total energy per unit volume. The symbol $\otimes$ denotes the tensor product of vectors.

At the boundary of the domain, a no-flow condition is imposed. In the two-dimensional case $\Omega = [0,1] \times [0,1], \mathbf{u} = (u_1, u_2)$

$$u_1(t,0,x_2) = u_1(t,1,x_2) = 0,\ u_2(t,x_1,0) = u_2(t,x_1,1) = 0.$$

And the initial conditions are given as follows:

$$\rho|_{t=0} = \rho^0(x) \geqslant 0, \mathbf{u}|_{t=0} = \mathbf{u}^0(x), e|_{t=0} = e^0(x) \geqslant 0, x \in \Omega.$$

We will assume that the initial conditions are consistent, i.e. if $\rho^0(x) = 0$, then $\mathbf{u}^0(x) = 0, e^0(x) = 0$.

For this problem, under the conditions of existence and differentiability of the functions ρ, $\mathbf{u}, e$, one can formally obtain the integral identity

$$\int\limits_{\Omega} e(t,x)dx = \int\limits_{\Omega} e(0,x)dx.$$

Further, we will assume that the solution of the original problem is differentiable. In this work we will construct a difference scheme that inevitably has a grid viscosity and that satisfies the grid analog of the energy inequality

$$\int\limits_{\Omega} e(t,x)dx \leqslant \int\limits_{\Omega} e(0,x)dx. \tag{2}$$

We will construct difference schemes on a uniform orthogonal grid. The approximation of the continuity and motion equations is constructed in [1]. The same approximations will be used here.

To approximate the energy equation, we perform transformations and replace the unknown function. We multiply the continuity equation by $\mathbf{u}^2/2$, multiply the equation of motion by $\mathbf{u}$ and subtract from the energy equation. Taking into account the equation of state, we obtain

$$\frac{\partial \rho\varepsilon}{\partial t} + \mathrm{div}[(\rho\varepsilon)\mathbf{u}] + (\gamma - 1)\rho\varepsilon \mathrm{div}\mathbf{u} = 0.$$

Let $\rho\varepsilon = q \geqslant 0$. Let's introduce a new unknown function $s^\gamma = q$. Then for s we get an equation similar to the continuity equation:

$$\frac{\partial s}{\partial t} + \mathrm{div} s\mathbf{u} = 0.$$

The pressure gradient, according to the equation of state and the assumption of differentiability of the solution of the original problem, is transformed to the form $\mathrm{grad} p = \gamma s \,\mathrm{grad} s^{\gamma-1}$.

3. Difference scheme for the continuity equation

Next, we will construct a difference scheme for this problem. The goal of the work is to obtain difference analogs of the non-negativity condition for the density function ρ and the function s, the conservatism condition

$$\int\limits_\Omega \rho(t,x)dx = \int\limits_\Omega \rho(0,x)dx, \int\limits_\Omega s(t,x)dx = \int\limits_\Omega s(0,x)dx, \forall t > 0$$

and the energy inequality (2).

Since the equations for ρ and s are the same, we will only define an approximation of the continuity equation. Using the notation from [1], we recall the approximation in two-dimensional case:

$$\rho_t + (\{\rho^{n+1}\}_1 u_1)_{x_1} + (\{\rho^{n+1}\}_2 u_2)_{x_2} = 0,$$

$$\{\rho^{n+1}\}_1 = \rho^{n+1} - h\rho^{n+1}_{\bar{x}_1} \max(0, \mathrm{sign}(u_1)) = [\rho^{n+1}]_1 - \frac{h}{2}\rho^{n+1}_{\bar{x}_1}\mathrm{sign}(u_1),$$
$$\{\rho^{n+1}\}_2 = \rho^{n+1} - h\rho^{n+1}_{\bar{x}_2} \max(0, \mathrm{sign}(u_2)) = [\rho^{n+1}]_2 - \frac{h}{2}\rho^{n+1}_{\bar{x}_2}\mathrm{sign}(u_2).$$

The bracket operators $\{.\}_1, \{.\}_2$ depend on the grid functions u_1, u_2.

The matrix $A\rho^{n+1} = (\{\rho^{n+1}\}_1 u_1)_{x_1} + (\{\rho^{n+1}\}_2 u_2)_{x_2}$ has the following properties: the diagonal contains non-negative numbers, the off-diagonal entries are non-positive numbers; the sum of the elements along a column is zero. Consider the matrix $B = (E + \tau A)^T$. It has non-negative numbers on its diagonal, non-positive numbers outside the diagonal, and has a strict diagonal dominance along the row. For a matrix with such a property, the Jacobi and Seidel iterative methods converge for any initial approximation. Let SLAE $Bx = b$ be solved by the Jacobi method with the initial approximation $x_0 = 0$ and the right-hand side vector b consisting of non-negative numbers. From the computational scheme of the Jacobi method

$$x_i^{n+1} = \frac{1}{B_{i,i}}(b_i - \sum_{k=1,k\neq i}^{M} B_{i,k}x_k^n), i = 1, 2, ..., M$$

it follows that $x_i^n \geqslant 0, i = 1, 2, ..., M, n = 1, 2, ...$ The limit vector will also be non-negative. Thus, for any non-negative vector b, the vector $x = B^{-1}b$ will be non-negative. This means that the matrix B^{-1} consists of non-negative numbers. Consequently, the matrix $(E + \tau A)^{-1} = (B^{-1})^T$ exists and consists of non-negative numbers.

The matrix A has the following property:

Lemma 1. *In two-dimensional case, for any given grid functions u_1, u_2 and for $\forall \tau > 0$*

$$\left\| \left(\frac{1}{\tau} E + A \right)^{-1} \right\|_1 = \tau.$$

Moreover, the sum of the elements of the matrix $\left(\frac{1}{\tau} E + A \right)^{-1}$ over any column is exactly equal to τ.

Note that the maximum along any row is achieved on the diagonal element, and this maximum is strict. The matrix elements along the row do not decrease monotonically up to the diagonal element, then they do not increase monotonically. This can be proved by directly calculating the elements of the matrix $\left(\frac{1}{\tau} E + A \right)^{-1}$, for example, using Cramer's rule. Such calculations are quite simple, but rather cumbersome, so a detailed proof is omitted here, since this property is not used in the sequel.

Theorem 1. *The difference scheme for the continuity equation $\rho_t + A(u_1, u_2)\rho^{n+1} = 0$ and the equation for the function s : $s_t + A(u_1, u_2)s^{n+1} = 0$ with any given grid functions u_1, u_2 has a unique solution, and if $\rho^0 \geqslant 0, s^0 \geqslant 0$, then $\rho^n \geqslant 0, s^n \geqslant 0$*

for $\forall n$. *The difference scheme is conservative, i.e.*

$$\sum_{i=0}^{N_1-1}\sum_{j=0}^{N_2-1} h_1 h_2 \rho_{ij}^n = \sum_{i=0}^{N_1-1}\sum_{j=0}^{N_2-1} h_1 h_2 \rho_{ij}^0.$$

Similar is true for function s *in two-dimensional case.*

From non-negativity and conservatism it follows that $\|\rho^n\|_{L_{1,h}}$ = const for $\forall n$. If u_1, u_2 are the given functions and $\rho^0 \geqslant 0$, then the obtained equality is a condition for weak stability of difference scheme.

For the function s, the approximation is exactly the same as for ρ. We will assume that the initial conditions are consistent, i.e. if $\rho^0 = 0$ at some point of the grid, then $s^0 = 0$ at the same point. In this case, grid points cannot arise during the transition to the next layer in time, where $s^1 \neq 0$ and $\rho^1 = 0$. For the next layers in time, the same applies.

4. Fully implicit nonlinear scheme

When approximating the equation of motion, the same principle of directed differences against the flow is used as when approximating the continuity equation. Let us consider a fully implicit nonlinear difference scheme, similar to that constructed in [1]:

$$\begin{gathered}
\rho_t + (\{\rho^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{\rho^{n+1}\}_2 u_2^{n+1})_{x_2} = 0,\\
(\rho u_1)_t + (\{\rho^{n+1} u_1^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{\rho^{n+1} u_1^{n+1}\}_2 u_2^{n+1})_{x_2} + \gamma s^{n+1}((s^{n+1})^{\gamma-1})_{\bar{x}_1} = 0,\\
(\rho u_2)_t + (\{\rho^{n+1} u_2^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{\rho^{n+1} u_2^{n+1}\}_2 u_2^{n+1})_{x_2} + \gamma s^{n+1})((s^{n+1})^{\gamma-1})_{\bar{x}_2} = 0,\\
s_t + (\{s^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{s^{n+1}\}_2 u_2^{n+1})_{x_2} = 0,
\end{gathered}$$

in two-dimensional case. The bracket operators $\{\cdot\}_*$ are defined by the functions u_1^{n+1}, u_2^{n+1} in two-dimensional case.

Further reasoning does not differ fundamentally from that of [1, 4]. There, the method of energy inequalities is used, and the calculations in [4] are detailed, although very cumbersome.

The difference scheme is investigated as follows. Since the scheme is nonlinear and implicit, it is necessary to verify the solvability of the problem at each step. For this, an iterative process, the Leray-Schauder principle, and a double limit transition are used.

We use the following version of the Leray-Schauder principle [3].

Let A *be a completely continuous operator in a separable normed space* F, *and let any possible solution* $X \in F$ *of the equation* $X + \alpha A(X) = 0$ *be uniformly bounded for* $\alpha \in (0, 1]$. *Then there exists at least one solution of the equation* $X + A(X) = 0$.

Theorem 2. *Let the function ρ^0 be strictly greater than zero at the initial moment of time. Then there exists a solution to the difference scheme.*

To complete the proof of the theorem, it remains to verify the validity of the energy inequality. As in [1], Young's inequality is used.

Here the theorem is formulated for a positive initial condition ρ^0. In general, this requirement is redundant. We can use the matching conditions for the velocity and internal energy, setting them equal to zero at the points where the density is zero, and not calculating them at the corresponding step. And when the density, which is calculated for all points, becomes nonzero, then at the next time step both the velocity and the internal energy are calculated at such points. This approach allows us to prove Theorem 3 for a wider class of problems. We had to deal with exactly this situation when modeling shallow water flows with a curved bottom. Namely, in the shallow water model, the continuity equation for the thickness of the water layer is obtained:

$$\frac{\partial h}{\partial t} + \mathrm{div} h\mathbf{u} = 0.$$

Here h is the thickness of the shallow water layer. And, as a result of the shallow water level fluctuations above the surface, islands may appear through which the flow cannot run. The function h degenerates, and the velocities should be set to zero. This approach was called the rule of internal boundary conditions.

5. Shifted grid scheme

For practical calculations, the considered scheme in the version of the linear implicit scheme has a drawback, since it does not preserve possible symmetries of flows present in the original problem.

Now, we will consider another difference scheme. In this scheme, the symmetry of difference relations is used if the grid functions ρ, u_1, u_2, s are considered on shifted grids.

For grids on which ρ, s are defined, the nodes of the uniform orthogonal grid are shifted to the centers of grid cells by half a step up and half a step to the right, for u_1 the grid is shifted by half a step up, for u_2 - to the right. The grid shifts are carried out without changing the numbering of the nodes.

We will assume that the initial conditions are consistent, i.e. at the grid points where $\rho^0 = 0$, the grid function $s = 0$. The conditions for the consistency of the initial conditions for the velocities are the same as in the Rule of Internal Boundary Conditions.

5.1. Internal boundary conditions rule for a fully implicit nonlinear scheme on shifted grids

At the computation points $[\rho^n_{i,j}]_1 = 0, [s^n_{i,j}]_1 = 0$, *the approximation of the first equation of motion is replaced by the internal boundary condition* $u^{n+1}_{1,i,j} = 0$, *at the points* $[\rho^n_{i,j}]_2 = 0, [s^n_{i,j}]_2 = 0$, *the approximation of the second equation of motion is replaced by the internal boundary condition* $u^{n+1}_{2,i,j} = 0$.

In two-dimensional case, we obtain a difference scheme

$$\rho_t + (\{\rho^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{\rho^{n+1}\}_2 u_2^{n+1})_{x_2} = 0,$$

$$([\rho]_1 u_1)_t + \frac{1}{2}(\{\rho^{n+1} u_1^{n+1}\}_1 u_1^{n+1})_{x_1} + \frac{1}{2}(\{\rho^{n+1}\}_1 < u_1^{n+1} >_1 u_1^{n+1})_{\bar{x}_1} +$$
$$+([\{\rho^{n+1}\}_2 u_2^{n+1}]_1 [u_1^{n+1}]_2)_{x_2} + \gamma [s^{n+1}]_1 ((s^{n+1})^{\gamma-1})_{\bar{x}_1} = 0,$$

$$([\rho]_2 u_2)_t + ([\{\rho^{n+1}\}_1 u_1^{n+1}]_2 [u_2^{n+1}]_1)_{x_1} +$$
$$+\frac{1}{2}(\{\rho^{n+1} u_2^{n+1}\}_2 u_2^{n+1})_{x_2} + \frac{1}{2}(\{\rho^{n+1}\}_2 < u_2^{n+1} >_2 u_2^{n+1})_{\bar{x}_2} +$$
$$+\gamma [s^{n+1}]_2 ((s^{n+1})^{\gamma-1})_{\bar{x}_2} = 0,$$

$$s_t + (\{s^{n+1}\}_1 u_1^{n+1})_{x_1} + (\{s^{n+1}\}_2 u_2^{n+1})_{x_2} = 0.$$

$$< u^{n+1} >_1 = \frac{u^{n+1}_{i+1,j} + u^{n+1}_{i,j}}{2} - \frac{h}{2}(u^{n+1})_{x_1} \mathrm{sign}(u^{n+1}_{ij}), < u^{n+1} >_2 =$$
$$= \frac{u^{n+1}_{i,j+1} + u^{n+1}_{i,j}}{2} - \frac{h}{2}(u^{n+1})_{x_2} \mathrm{sign}(u^{n+1}_{ij}).$$

The first equation of motion is approximated at the points where $[\rho^n]_1 > 0$. At the points where $[\rho^n]_1 = 0$, the function $u_1^{n+1} = 0$ is considered as given. The second equation of motion is approximated at the points where $[\rho^n]_2 > 0$. At the points where $[\rho^n]_2 = 0$, the function $u_2^{n+1} = 0$ is considered as given. And if such points exist, then the problem has the given internal boundary conditions, i.e. conditions of no-flow in one of directions.

Now let us explain why such an approximation was chosen in two-dimensional case.

$$\frac{\partial(\rho v_1 u_2)}{\partial x_2} \sim ([\{\rho^{n+1}\}_2 u_2^{n+1}]_1 [v_1^{n+1}]_2)_{x_2}.$$

This approximation does not include grid viscosity, but may be poor, since the tridiagonal matrix of this approximation does not necessarily have a non-negative diagonal element and the rest of its elements non-positive. This approximation can be corrected by the same rule by which the approximation of the continuity equation was constructed, i.e. by using differences against the flow:

$([\{\varrho\}_2 u_2]_1([v_1]_2 - \frac{h_2}{2}(v_1)_{\bar{x}_2}\mathrm{sign}([\{\varrho\}_2 u_2]_1)))_{x_2}$. This approximation may be two-point or even one-point and not contain the function sign. In terms of indices, this approximation has the form

$$\frac{1}{2}\left(-|w_{i,j+1}| + w_{i,j+1}\right) v_{1i,j+1} +$$

$$+\frac{1}{2}\left(w_{i,j+1} + |w_{i,j+1}| - w_{i,j} - |w_{i,j}|\right) v_{1i,j} + \frac{1}{2}\left(-w_{i,j} + |w_{i,j}|\right) v_{1i,j-1},$$

where $w_{i,j} = [\{\varrho\}_2 u_2]_1$ is a known function that determines the problem matrix for the first velocity component.

Theorem 3. *Let $\rho^0 \geqslant 0$ and the initial conditions for s and the grid velocity be consistent at the grid points where $\rho^0 = 0$. The solution of the difference scheme II with internal boundary conditions exists, the grid density and the function s are non-negative, the grid analogue of the law of conservation of mass is satisfied, the grid analogue of the law of conservation of the "radical of internal energy" is satisfied, and the grid energy inequality is satisfied.*

Advantages of the scheme:

1. Non-negativity of the density, the law of conservation of mass is satisfied: $\|\rho^n\|_{L_{1,h}(\Omega)} = \mathrm{const}$;
2. Non-negativity of internal energy, the law of conservation of the radical of internal energy is satisfied: $\|\sqrt[\gamma]{q^n}\|_{L_{1,h}(\Omega)} = \mathrm{const}$;
3. Grid energy inequality is satisfied. The scheme is dissipative.
4. If at some computation point the density becomes positive, then it will remain positive at all subsequent time steps. If the density is zero, then all other unknowns should be zeroed according to the rule of internal boundary conditions.

Remark 1. *In practical calculations, it is impossible to use a nonlinear implicit scheme, so a linear implicit scheme and an internal iteration process are usually used at each time step. Internal iteration processes with factorization of the transition operator to the next time step have proven themselves well.*

In the equation of motion of the original problem, the pressure gradient is written in a non-conservative form, so we initially assume differentiability of the solution to the original problem. In this case, the problems will be equivalent. Thus, the considered scheme is proposed for calculating flows without discontinuities or with low-intensity discontinuities.

In the work, a scheme for a model problem without external forces is considered. For real problems, the same approximations of differential operators can be used. These approximations can be extended to curvilinear non-orthogonal grids, to non-simply connected computational domains and to the case of three spatial coordinates.

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Fariz B. Imranov
Department of Electronic Academy of the Presidium of the NAS of Azerbaijan, Baku, Azerbaijan
E-mail: farizimranov@yandex.ru

Aleksandr G. Sokolov
Moscow State University, Moscow, Russia
E-mail: shurunya@mtu-net.ru

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