COMPARATIVE ANALYSIS OF THE QUALITY OF TWO-AND THREE-LAYER DIFFERENCE SCHEMES OF THE SECOND ORDER

V.I.MAZHUKIN[1,2], A.V. SHAPRANOV[1,2], E.N. BYKOVSKAYA[1]

[1] Keldysh Institute of Applied Mathematics of Russian Academy of Sciences (KIAM RAS)
4 Miusskaya square, 125047 Moscow, Russia
e-mail: vim@modhef.ru, web page: http://www.keldysh.ru

[2] National Research Nuclear University Moscow Engineering Physics Institute (NRNU MEPhi)
31 Kashirskoe shosse, 115409, Moscow, Russia

Summary. Using the example of a numerical solution of a model problem with a nonlinear Burgers equation, the quality of the approximation of the original equation by two and three-layer difference schemes written on grids with fixed and moving nodes is studied. Modeling with the subsequent analysis of its results has shown that in the Cartesian coordinate system the quality of the numerical solution essentially depends on the quality of the finite-difference approximation used for the initial equation. The application of the two-layer Crank-Nicholson scheme and the three-layer difference scheme of the Cabaret type with the second order of approximation formulated in the Cartesian coordinate system showed that the three-layer difference schemes have a distinct advantage and give a solution of higher quality, except for regions with large gradients. The application of an arbitrary non-stationary coordinate system made it possible to implement a dynamic adaptation of the grid in which the distribution of nodes is dependent and controlled by the sought solution, which makes it possible to automatically adjust the calculated grid in such a way that the approximation error turns out to be minimal practically regardless of the quality of the original difference scheme. The numerical solution of the nonlinear Burgers equation with the help of two and three-layer difference schemes on a dynamically adapting grid showed virtually complete coincidence of the calculations with each other, a good agreement with the exact solution with complete absence of oscillations in the solution. The calculation grid contained the number of nodes (n = 25) by two orders of magnitude smaller than the grid with fixed nodes.

1 INTRODUCTION

The numerical solution of the equations of continuum mechanics, which describe convection-diffusion processes with the predominance of the convective transport mechanism, is one of the fundamental problems of computational mathematics. The main difficulties of the computational process are due to the error that arises when differential equations are approximated by difference schemes. The approximation error is manifested in the form of dissipative and dispersive properties of finite-difference schemes. Depending on the relationship between these properties in the solution, not only quantitative, but also qualitative distortions can occur.

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Such computational features are the most completely investigated and generalized in the systems of linear and nonlinear equations of hyperbolic type. These include the equations of gas dynamics [1], elasticity theory [2], shallow water [3,4], etc. For many years of research a large number of finite-difference schemes have been developed [5-9] for the solution of these equations, having their own advantages and disadvantages. It is known that classical finite-difference schemes with the first order of approximation for the equations of convective transport in Euler variables have too much dissipation, which leads to a strong smoothing of the solution in the regions of local extrema. The schemes of higher (2nd and higher) order according to the theorem of S.K. Godunov [10] are not monotonic due to a high approximation dispersion, which often causes the appearance of parasitic oscillations in the regions of large solution gradients. As a result, classical difference schemes can not always provide the necessary accuracy of numerical solutions.

The dissipative and dispersion properties of classical difference schemes are improved in various ways. A decrease in the scheme dissipation can be achieved by increasing the order of approximation [8], and for the monotonization of the solution, the methods of artificial viscosity [7] and nonlinear correction [11] are usually used. Recently, the methods for constructing nonlinear difference schemes (so-called high resolution algorithms) that improve the dissipative and dispersive properties of classical linear difference schemes with the help of nonlinear correction of fluxes have become most widely used. When constructing improved nonlinear schemes of high accuracy order, the dissipative difference schemes of Godunov [10] or Lax-Wendroff [12] are used as the initial ones.

In one of the first papers [13], the construction of a high-resolution scheme (the Flux Corrected Transport (FCT) method) was achieved by reducing the dissipation in the original low-dispersion scheme (the first-order Godunov scheme [10]), introducing antidiffusion fluxes while preserving the boundedness of the solution [14]. Another example of constructing high-resolution schemes is higher order approximation schemes based on the principle of non-increase of the total variation of the solution (TVD - Total Variation Diminishing) [11,15,16]. In this approach, to fight with numerical oscillations, an increase in the order of approximation is used, which is achieved by adding delimiters to the difference scheme in such a way that the scheme possesses a high order on smooth solutions and retains monotonicity in the regions of strong discontinuity. Methods for constructing difference schemes with low dispersion also include the ENO (essentially non-oscillatory) and WENO (weighted essentially non-oscillatory) methods [17-20]. These methods, like the TVD methods, are used to achieve a more subtle balance between dispersion and dissipation errors. Increasing the order of approximation in these schemes is achieved by increasing the computational template. Most highly accurate methods based on explicit wide-template difference schemes [21, 22] of an increased (up to the 12th [23]) approximation are found in shallow water problems [24] and aeroacoustics [25, 26]. However, the use of wide-scale schemes faces a number of difficulties associated with setting the boundary conditions, modifying the templates near the boundaries, and the sensitivity of the schemes used to the degree of homogeneity of the calculated grids.

The use of wide-template schemes is not the only way to obtain good dissipative and dispersion properties. Another direction for improving the properties of difference schemes was formulated in [27], [28]. On the example of the solution of the one-dimensional convection transfer equation, explicit linear 3-layer difference schemes with improved dispersive and dissipative properties were shown in these papers and are known as the

Upwind Leapfrog [27] and Cabaret (Compact Accurately Boundary-Adjusting High-REsolution Technique) schemes [28]. The Cabaret scheme is designed taking into account the results of the Upwind Leapfrog scheme. It was based on a new formulation of the compact Upwind Leapfrog scheme of the second order, which is achieved by introducing independent conservative and flux variables. The scheme proposed in the first papers [28], [29] was further developed in [30], [31]. The necessary monotonization of the solutions in the regions of large gradients was achieved with the help of a simple algorithm of nonlinear correction of fluxes based on the maximum principle [30].

A distinctive feature of the Cabaret scheme, in comparison with the most high-resolution schemes, is that it is completely discrete in space and time (x, t), has a second order in x and t ($O(\Delta x^2 + \Delta t^2)$) and, all improved properties are obtained on the least possible compact difference template. Later, the Cabaret scheme was generalized to the cases described by quasilinear hyperbolic equations [32], [33] and the equations of gas dynamics in the one-dimensional and two-dimensional approximation [34].

The brief overview shows that the problem of finding new ways to improve the dissipative and dispersive properties of the difference schemes used to solve the problems of fluid and gas mechanics remains open and is still relevant.

The purpose of this publication is to demonstrate a different approach to improving the dissipative-dispersion properties of difference schemes with a second order of approximation. The achievement of this goal is carried out using the method of dynamic adaptation [35], [36], in which the controlled distribution of nodes of the grid at each time is achieved by the sought solution. A complete matching of the motion of the grid nodes with the evolution of the solution leads to a decrease in the dissipation and to the complete zeroing of the dispersion of the difference scheme. Demonstration of the possibilities of the approach is carried out using the example of a numerical solution of the Burgers equation. The effectiveness of this approach is determined by comparing the results of the solution of the Burgers equation with the use of two-layer difference schemes of Crank-Nicolson and three-layered Cabaret type.

2 STATEMENT OF THE PROBLEM

A number of mathematical models that form the basis of the problems of fluid and gas mechanics are reduced to the convection-diffusion problems. These models describe two basic mechanisms of energy and substance transfer: diffusion and convection. Depending on the external conditions, each of the mechanisms may have a dominant influence. To estimate the predominance of a particular process, one usually uses dimensionless parameters, the so-called Peclet number (*Pe*) or Reynolds number (*Re*). At $Pe << 1$ ($Re << 1$) the diffusion process dominates in the system, and for $Pe >> 1$ ($Re >> 1$) the convective transfer predominates. In the case of strong dominance of the convective transport mechanism, a class of singularly perturbed nonlinear mathematical models with a small parameter $\mu = Pe^{-1}$ or $\mu = Re^{-1}$ with the highest derivative is obtained. Nonstationary singularly perturbed models on the basis of the Burgers-Buckley-Leverett equations allow the emergence of regions of strong change in the solution propagating in the form of various fronts and transition layers.

From a computational point of view, singularly perturbed problems are referred to as difficult problems to be solved. In particular, the difference schemes used to approximate the convection-diffusion equations, as a rule, have a strong dispersion, for the suppression of which special measures are applied. In computing practice, a wide application as a test

problem for the problems of the boundary layer, parabolized and complete Navier-Stokes equations has the Burgers equation with the corresponding boundary conditions. The complete non-linear Burgers equation contains a quadratic nonlinearity in the convective summand and a linear viscosity on the right-hand side. The solution of the Burgers equation, with a coefficient of viscosity tending to zero, can contain both strong (shock waves) and weak discontinuities, which allows one to analyze all the singularities of the solution for arbitrary initial data.

Taking into account the initial and boundary conditions, the Burgers problem is formulated as follows:

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(\frac{u^2}{2}\right)=\mu\frac{\partial^2 u}{\partial x^2} \tag{1}$$

$$t>0,\quad x_0<x<x_R$$

$$t=0:\quad u(x,0)=u_0(x),\quad x_0<x<x_R \tag{2}$$

$$x=x_0:\quad g_0\left(x,t,u(x),\frac{\partial u}{\partial x}\right)=0,\quad x=x_R:\quad g_R\left(x,t,u(x),\frac{\partial u}{\partial x}\right)=0 \tag{3}$$

where the coefficient $\mu(x)$ has the meaning of viscosity, $u_0(x)$, $g_0\left(x,t,u(x),\frac{\partial u}{\partial x}\right)$, $g_R\left(x,t,u(x),\frac{\partial u}{\partial x}\right)$ are given functions.

3 ONE-PARAMETER FAMILIES OF TWO- AND THREE-LAYER DIFFERENCE SCHEMES OF THE SECOND, $O(\Delta t^2+h^2)$

Consider the calculation space $\Omega_{x,t}$, in which a Cartesian coordinate system is set with variables (x,t). In the space $\Omega_{x,t}$ consider a computational grid $\omega_{\Delta x}^{\Delta t}$, in which for convenience we use nodes with integer and half-integer indices:

$$\omega_{\Delta x}^{\Delta t}=\left(x_m,t^k\right),\left(x_{m+\frac{1}{2}},t^{k+\frac{1}{2}}\right): x_{m+1}=x_m+\Delta x_m,\ x_{m+\frac{1}{2}}=x_m+\frac{\Delta x_m}{2},$$

$$t^{k+1}=t^k+\Delta t^k,\ t^{k+\frac{1}{2}}=t^k+\frac{\Delta t^k}{2},\quad m=\overline{0,N};\ k=\overline{0,J}$$

The one-parameter family of two-layer schemes for the Burgers equation, written out on a computational grid with fixed nodes, has the form:

$$\frac{u_{m-1/2}^{k+1}-u_{m-1/2}^{k}}{\Delta t^{j}}=\sigma\left[-\frac{1}{2\Delta x}\left(\frac{(u_{m+1/2}^{k+1})^2}{2}-\frac{(u_{m-3/2}^{k+1})^2}{2}\right)+\frac{\mu}{\Delta x}\left(\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta x}-\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta x}\right)\right]+$$

$$+(1-\sigma)\left[-\frac{1}{2\Delta x}\left(\frac{(u_{m+1/2}^{k})^2}{2}-\frac{(u_{m-3/2}^{k})^2}{2}\right)+\frac{\mu}{\Delta x}\left(\frac{u_{m+1/2}^{k}-u_{m-1/2}^{k}}{\Delta x}-\frac{u_{m-1/2}^{k}-u_{m-3/2}^{k}}{\Delta x}\right)\right] \quad (4)$$

where σ is the weight factor, determining the degree of implicitness of the difference scheme, $0<\sigma<1$. For $\sigma = 0.5$ we have a symmetric Crank-Nicolson scheme with the second order of approximation $O(\Delta t^2+\Delta x^2)$.

Using the approach to constructing an implicit three-layer difference scheme for the linear transport equation, presented in [34], we write out a family of three-layer implicit schemes of Cabaret type, consisting of 3 parts, for the Burgers equation (1).

Part one – time transition $u_{m-1/2}^{k} \to u_{m-1/2}^{k+1/2}$

$$\frac{u_{m-1/2}^{k+1/2}-u_{m-1/2}^{k}}{\Delta\tau/2}+\sigma_1\frac{1}{\Delta x}\left(\frac{\left(u_m^{k+1}\right)^2}{2}-\frac{\left(u_{m-1}^{k+1}\right)^2}{2}\right)+(1-\sigma_1)\frac{1}{\Delta x}\left(\frac{\left(u_m^{k}\right)^2}{2}-\frac{\left(u_{m-1}^{k}\right)^2}{2}\right)=$$

$$=(1-\sigma_2)\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta x}\right)\right]+$$

$$+\sigma_2\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k}-u_{m-1/2}^{k}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k}-u_{m-3/2}^{k}}{\Delta x}\right)\right]$$

Part two – extrapolation

$$u_m^{k+1}=\begin{cases}2u_{m-1/2}^{k+1/2}-u_{m-1}^{k}, & for \quad u_{m-1/2}^{k+1/2}>0;\\ u_{m-1/2}^{k+1/2}+u_{m+1/2}^{k+1/2}-u_m^{k}, & for \quad u_{m-1/2}^{k+1/2}=0;\\ 2u_{m+1/2}^{k+1/2}-u_{m+1}^{k}, & for \quad u_{m-1/2}^{k+1/2}<0;\end{cases} \quad (5)$$

Part three – time transition $u_{m-1/2}^{k+1/2} \to u_{m-1/2}^{k+1}$

$$\frac{u_{m-1/2}^{k+1}-u_{m-1/2}^{k+1/2}}{\Delta\tau/2}+(1-\sigma_1)\frac{1}{\Delta x}\left(\frac{\left(u_m^{k+1}\right)^2}{2}-\frac{\left(u_{m-1}^{k+1}\right)^2}{2}\right)+\sigma_1\frac{1}{\Delta x}\left(\frac{\left(u_m^{k}\right)^2}{2}-\frac{\left(u_{m-1}^{k}\right)^2}{2}\right)=$$

$$=\sigma_2\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta x}\right)\right]+$$

$$+(1-\sigma_2)\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta x}\right)\right]$$

For $\sigma_1 = \sigma_2 = 0.5$ we obtain a scheme with the second order of approximation $O(\Delta t^2+\Delta x^2)$.

4 ALGORITHM OF NUMERICAL SOLUTION

The system of difference equations (4) was solved by the Newton iterative method with the use of a three-diagonal sweep method at each iteration [37] to solve a system of linear algebraic equations. The step of integration $\Delta\tau^k$ was selected automatically based on the specified accuracy and the maximum number of iterations

Algorithm for the numerical solution of an implicit three-layer scheme (5) with $\sigma_1 = \sigma_2 = 0.5$ consists of three stages.

At the first stage, a system of nonlinear algebraic equations is solved (6), from where the conservative variables are found $u_{m-1/2}^{k+1/2}$ during the first half-timestep.

$$\begin{aligned}
&\frac{u_{m-1/2}^{k+1}-u_{m-1/2}^{k+1/2}}{\Delta\tau/2}+\frac{1}{2}\frac{1}{\Delta x}\left(\frac{\left(u_m^{k+1}\right)^2}{2}-\frac{\left(u_{m-1}^{k+1}\right)^2}{2}\right)+\frac{1}{2}\frac{1}{\Delta x}\left(\frac{\left(u_m^{k}\right)^2}{2}-\frac{\left(u_{m-1}^{k}\right)^2}{2}\right)=\\
&=\frac{1}{2}\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta x}\right)\right]+\\
&+\frac{1}{2}\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta x}\right)\right]
\end{aligned} \tag{6}$$

At the second stage, extrapolation of the flux variables occurs within the space-time cells.

$$u_m^{k+1}=\begin{cases}2u_{m-1/2}^{k+1/2}-u_{m-1}^{k}, & \text{for} \quad u_{m-1/2}^{k+1/2}>0;\\ u_{m-1/2}^{k+1/2}+u_{m+1/2}^{k+1/2}-u_m^{k}, & \text{for} \quad u_{m-1/2}^{k+1/2}=0;\\ 2u_{m+1/2}^{k+1/2}-u_{m+1}^{k}, & \text{for} \quad u_{m-1/2}^{k+1/2}<0;\end{cases} \tag{7}$$

At the third stage, the system of the difference equations is solved, from which the conservative variables $u_{m-1/2}^{k+1}$ are found at the new time layer [29], [30]:

$$\begin{aligned}
&\frac{u_{m-1/2}^{k+1}-u_{m-1/2}^{k+1/2}}{\Delta\tau/2}+\frac{1}{2}\frac{1}{\Delta x}\left(\frac{\left(u_m^{k+1}\right)^2}{2}-\frac{\left(u_{m-1}^{k+1}\right)^2}{2}\right)+\frac{1}{2}\frac{1}{\Delta x}\left(\frac{\left(u_m^{k}\right)^2}{2}-\frac{\left(u_{m-1}^{k}\right)^2}{2}\right)=\\
&=\frac{1}{2}\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta x}\right)\right]+\frac{1}{2}\frac{\mu}{\Delta x}\left[\left(\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta x}\right)-\left(\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta x}\right)\right]
\end{aligned} \tag{8}$$

Just as in the case of a two-layer scheme, the iterative Newton method was used to solve the difference schemes (6), (8) using sweeping at each iteration. The integration step $\Delta\tau^k$ was selected automatically based on the specified accuracy and the maximum number of iterations. To achieve monotonicity of the solution in the presence of large gradients, after each iteration, the solution was monotonized on the basis of the maximum principle:

$$u_m^{s+1} = \begin{cases} min(u_{m-1}^k, u_m^k), & for \quad u_{m-1/2}^{k+1/2} > 0, u_m^{s+1} \le min(u_{m-1}^k, u_m^k); \\ max(u_{m-1}^k, u_m^k), & for \quad u_{m-1/2}^{k+1/2} > 0, u_m^{s+1} \ge max(u_{m-1}^k, u_m^k); \\ u_m^{s+1}, & for \quad u_{m-1/2}^{k+1/2} > 0, min(u_{m-1}^k, u_m^k) \le u_m^{s+1} \le max(u_{m-1}^k, u_m^k); \\ min(u_{m+1}^k, u_m^k), & for \quad u_{m-1/2}^{k+1/2} < 0, u_m^{s+1} \le min(u_{m+1}^k, u_m^k); \\ max(u_{m+1}^k, u_m^k), & for \quad u_{m-1/2}^{k+1/2} < 0, u_m^{s+1} \ge max(u_{m+1}^k, u_m^k); \\ u_m^{s+1}, & for \quad u_{m-1/2}^{k+1/2} < 0, min(u_{m+1}^k, u_m^k) \le u_m^{s+1} \le max(u_{m+1}^k, u_m^k); \end{cases} \quad (9)$$

where s - is the iteration number.

5 MODELING AND ANALYSIS OF THE QUALITY OF TWO- AND THREE-LAYER DIFFERENCE SCHEMES ON THE GRIDS WITH FIXED NODES

The developed difference schemes (4), (6-9) were used to perform a series of calculations with subsequent comparison and an analysis of the quality of the scheme properties. As a test problem, we considered a nonlinear equation (1) with an initial condition in the form of an asymmetric sinusoid

$$u_0(x) = u(x,0) = sin(2\pi x) + 0.5\, sin(\pi x) \quad (10)$$

and boundary conditions:

$$u(x_0,t) = u(x_R,t) = 0 \quad (11)$$

The calculations were carried out on a grid with the same number of nodes – $N = 2500$. The value of μ parameter was chosen from the range $\mu \in \{10^{-3} \div 10^{-6}\}$.

Modeling showed that two half-waves of the sinusoid moving towards each other form a steep front, the thickness of which is determined by the value of the parameter μ. The use of the two-layer Crank-Nicolson scheme (5) showed that the first parasitic oscillations on the upper part of the front appear at $\mu=10^{-3}$ (Fig. 1a). The solution $u(x)$ obtained from the three-layer scheme with the flux correction (6) – (9) does not have any oscillations (Fig. 1b).

Further growth of the gradient of the solution, caused by a decrease in the parameter $\mu = 10^{-4}$ -10^{-6} leads to an increase in parasitic oscillations in solutions obtained from a two-layer scheme (5), (Fig.2 – 4), which testifies to the deterioration of the dispersion properties of the scheme from which the three-layer scheme (6) - (9) is free, using the procedure for monotonization of the solution, over the whole range of the values of the parameter μ (Fig.5).

Thus, the three-layer difference schemes of the Cabaret type, written out on the computational grids with fixed nodes, have a distinct advantage in the dispersion properties over the two-layer Crank-Nicolson schemes.

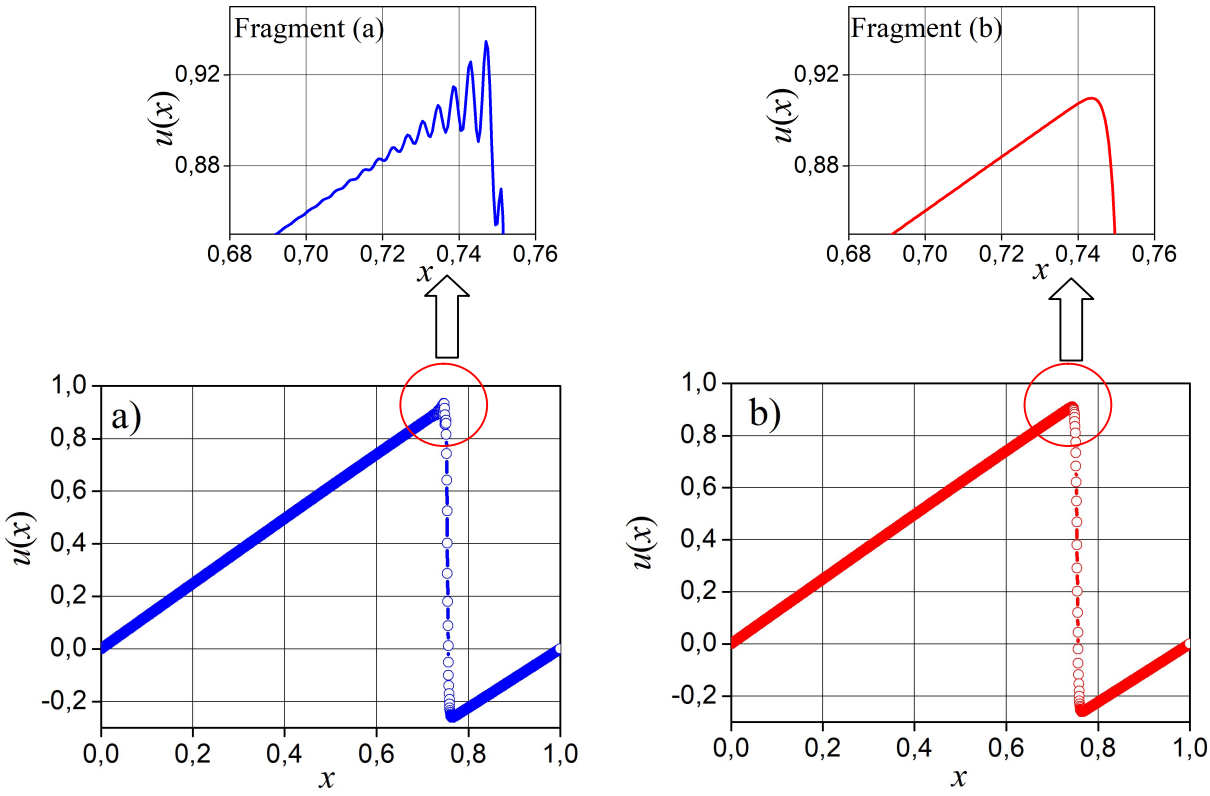

Fig. 1. Two-layer (a) and three-layer (b) schemes, $\mu=10^{-3}$

However, as noted in paper [34], the monotonization of the solution after each iteration in the region of large gradients leads to a deviation of the result from the exact solution of the original system of non-linear difference equations and can hinder the convergence of the iterative process.

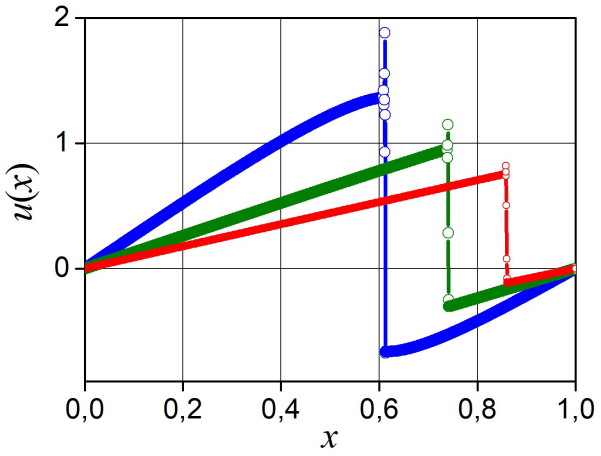

Fig. 2. Two-layer scheme, $\mu=10^{-4}$. Spatial profiles of the solution *u(x)* at the moments $t_{1\text{-}3}$ = 0.25, 0.63, 1.0

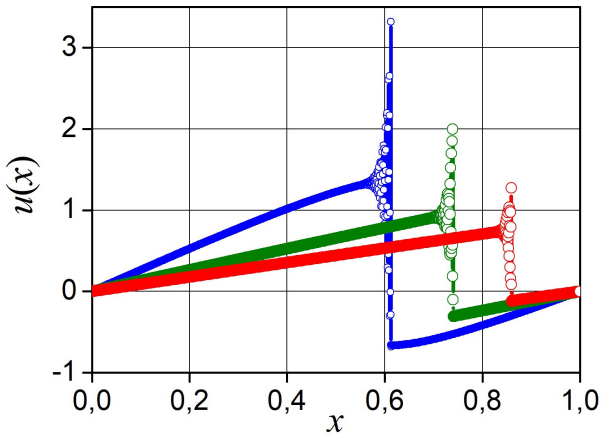

Fig. 3. Two-layer scheme, $\mu=10^{-5}$. Spatial profiles of the solution $u(x)$ at the moments $t_{1\text{-}3}$ = 0.25, 0.63, 1.0

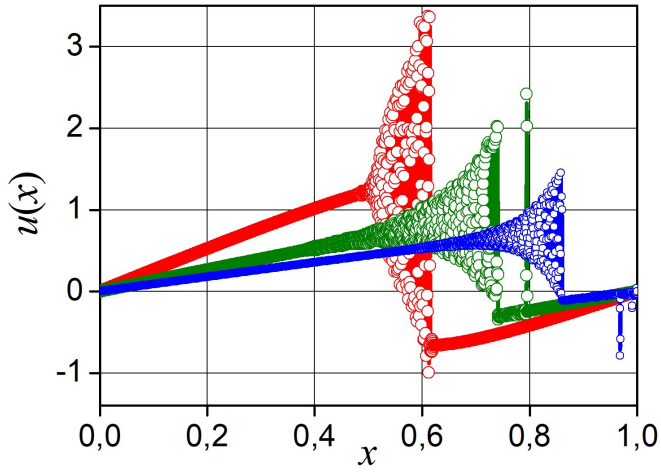

Fig. 4. Two-layer scheme, $\mu=10^{-6}$. Spatial profiles of the solution $u(x)$ at the moments $t_{1\text{-}3}$ = 0.25, 0.63, 1.0

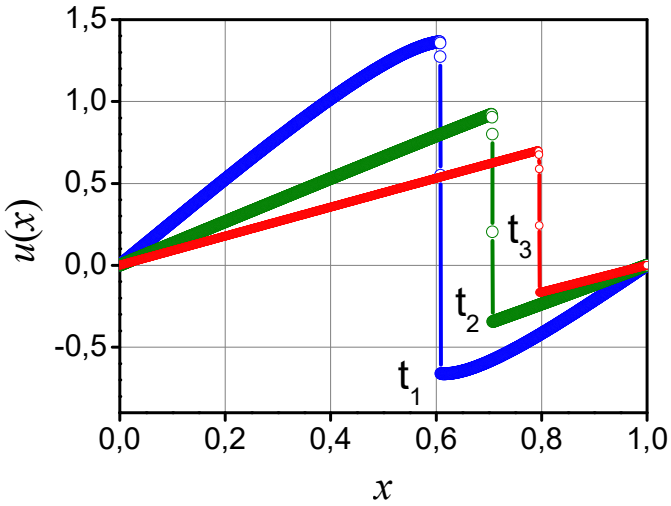

Fig. 5. Three-layer scheme, $\mu=10^{-4}$,. Spatial profiles of the solution $u(x)$ at the moemnts $t_{1\text{-}3}$ = 0.25, 0.63, 1.0

In this model problem (1), (10), (11), this defect is most clearly manifested in the slowing down of the motion of the solution front in comparison with the front of the exact solution [1] (Fig. 6a, b). The deceleration depends on the value of the parameter μ. The greatest lag is observed at $\mu = 10^{-3}$ and noticeably decreases at $\mu = 10^{-4}$, $\mu = 10^{-5}$.

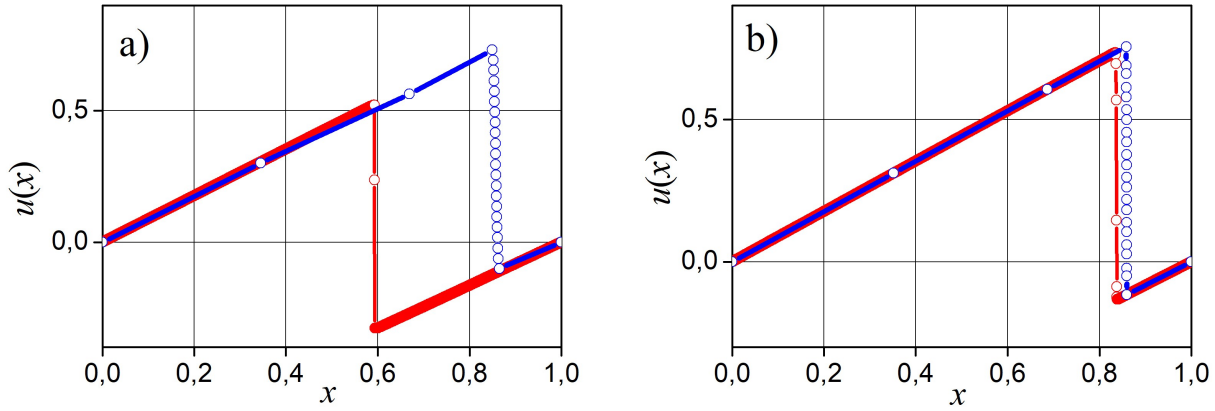

Fig. 6. Exact solution (blue line with symbols) and the solution obtained using the three-layer scheme (red line with symbols) for (a) -μ=10^{-3}, (b) - μ=10^{-4}.

The deviation from the exact solution in the region of large gradients is caused by the use of nonlinear correction of the fluxes, which is confirmed by comparing the results of calculations performed with monotonization of the solution and without it (Fig. 7 a, b). The front of the solution without the monotonization process is noticeably ahead of the front with monotonization. This indicates that the monotonization procedure used, despite the algorithmic simplicity, is not sufficiently flexible. Thus, the approach to improving the quality of the solution using difference schemes proposed in [28] - [34] is not free from certain shortcomings.

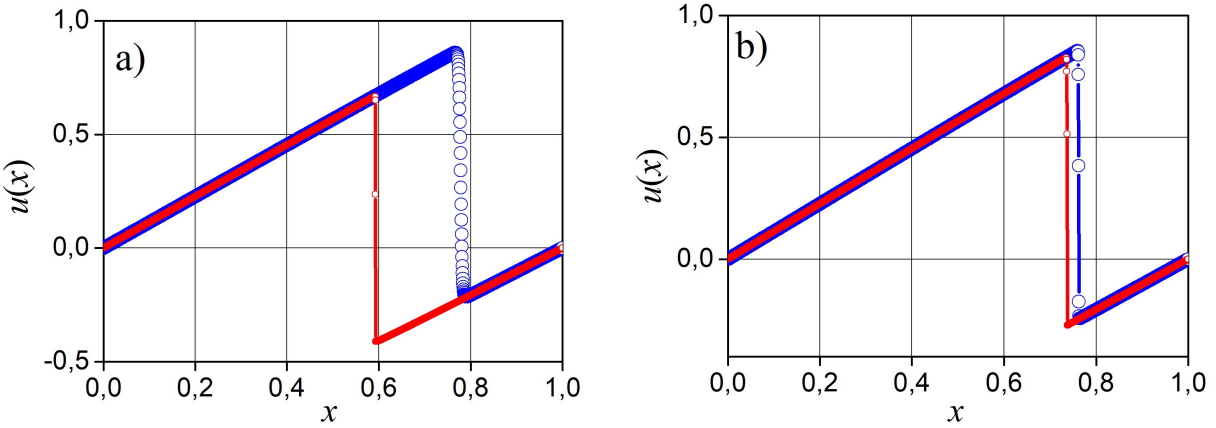

Fig. 7. The solution obtained using the three-layer scheme with monotonization (red line with symbols) and without monotonization (blue line with symbols) for (a) - μ=10^{-3}, (b) - μ=10^{-4}.

In the present paper, as an alternative, the reduction in the approximation error is proposed to be carried out using the method of dynamic adaptation of computational grids [35], [36], [38], [39]. The dynamic adaptation method was widely used to solve one-dimensional gasdynamic problems [40] - [45], one-dimensional and two-dimensional equations of parabolic type [46] - [49], one- and two-dimensional Stefan problems with moving phase boundaries [50] - [56] and a number of problems of laser action on matter [57] - [61].

6 MODELING AND ANALYSIS OF THE QUALITY OF THE TWO- AND THREE-LAYER DIFFERENCE SCHEMES ON THE GRIDS WITH MOVING NODES

The dynamic adaptation method is based on the procedure for transition from physical space $\Omega_{x,t}$ with a Cartesian coordinate system and variables (x,t) to some calculation space $\Omega_{q,\tau}$ with an arbitrary non-stationary coordinate system and variables (q,τ). The arbitrariness of a non-stationary coordinate system means that the speed of this coordinate system is unknown beforehand and must be determined in the course of the solution. The transition to an arbitrary nonstationary coordinate system makes it possible to formulate the problem of constructing and adapting computational grids at a differential level, because of this, in the resulting mathematical model, part of the differential equations describes physical processes, and the other describes the behavior of grid nodes [35], [40]. This allows adapting grids to various features of the solution, such as: large gradients [35], [36], [39] moving boundaries [48] - [52] and discontinuous solutions [40], [43] - [45].

The transition to an arbitrary non-stationary coordinate system is carried out by means of automatic transformation of coordinates with the help of the sought solution. The partial derivatives of the independent variables in the transition from one system to another are related by the following expressions:

$$\frac{\partial \cdot}{\partial t}=\frac{\partial \cdot}{\partial \tau}+\frac{Q}{\psi}\frac{\partial \cdot}{\partial q}\ ; \qquad \frac{\partial \cdot}{\partial x}=\frac{1}{\psi}\frac{\partial \cdot}{\partial q}; \qquad \frac{\partial^2 \cdot}{\partial x^2}=\frac{1}{\psi}\frac{\partial \cdot}{\partial q}\frac{1}{\psi}\frac{\partial}{\partial q} \tag{12}$$

where $\psi=\partial x/\partial q$ is the Jacobian of inverse transformation, the function Q characterizes the speed of motion of an unsteady coordinate system, is unknown in advance and is to be determined.

Using the relations (12) we represent the differential model (1) in the variables (q,τ):

$$\frac{\partial u}{\partial \tau}+\frac{Q}{\psi}\frac{\partial u}{\partial q}+\frac{1}{\psi}\frac{\partial}{\partial q}\left(\frac{u^2}{2}\right)=\frac{\mu}{\psi}\frac{\partial}{\partial q}\frac{1}{\psi}\frac{\partial u}{\partial q} \tag{13}$$

$$\frac{\partial x}{\partial \tau}=-Q \tag{14}$$

where (14) is the equation of inverse transformation with transformation function Q. The equation (14) is used to construct the grid that adapts to the solution. Its difference analog describes the dynamics of grid nodes, while the function Q realizes controlled movement of grid nodes, coordinated with the dynamics of the sought solution. The coordination is achieved by introducing a dependence of the function Q on the sought solution. Optimal transformation function Q, which ensures the complete coherence of the adaptation

mechanism with the desired solution, is determined from the quasi-stationary principle [36], [39], [48].

The meaning of the principle of quasi-stationarity lies in the requirement of transition to a non-stationary coordinate system in which the time derivatives of the solution are close to or equal to zero: $\partial u/\partial\tau = 0$. When this condition is satisfied, the equation (13) takes the form

$$\frac{Q}{\psi}\frac{\partial u}{\partial q}+\frac{1}{\psi}\frac{\partial}{\partial q}\left(\frac{u^2}{2}\right)=\frac{\mu}{\psi}\frac{\partial}{\partial q}\frac{1}{\psi}\frac{\partial u}{\partial q} \tag{15}$$

and serves to determine the function Q:

$$Q=-\left(u-\frac{\partial}{\partial q}\left(\frac{\mu}{\psi}\right)-\frac{\mu}{\psi}\left(\frac{\partial^2 u}{\partial q^2}\right)\left(\frac{\partial u}{\partial q}+re\right)^{-1}\right) \tag{16}$$

where $re << 1$ is the regularizer that prevents the first derivative from going to zero. The third term in (16) does not play any important role and can be ignored.

6.1 Differential approximation of difference schemes

By analyzing the differential approximation of the three-layer difference scheme, we show that the function found is optimal in the sense of the quality of the solution with a minimal number of grid nodes.

We introduce in the computational space $\overline{\Omega}_{q,\tau}$ a computational grid $\omega_{\Delta q}^{\Delta\tau}$:

$$\omega_{\Delta q}^{\Delta\tau}=\left(\begin{array}{l}\left(q_m,\tau^k\right);\quad q_{m+1}=q_m+\Delta q,\quad \tau^{k+1}=\tau^k+\Delta\tau^k, q_{m+\frac{1}{2}}=q_m+\dfrac{\Delta q}{2},\quad t^{k+\frac{1}{2}}=t^k+\dfrac{\Delta t^k}{2}\\ m=0,1,\ldots N\text{-}1,\quad k=0,1,\ldots,J\end{array}\right).$$

and consider the first part of the three-layer difference scheme for equation (15)

$$\begin{aligned}&\frac{1}{\Delta q}\left(\frac{(u_m^{k+1})^2}{2}-\frac{(u_{m-1}^{k+1})^2}{2}+Q_m^{k+1}u_m^{k+1}-Q_{m-1}^{k+1}u_{m-1}^{k+1}\right)+\frac{1}{\Delta q}\left(\frac{(u_m^{k})^2}{2}-\frac{(u_{m-1}^{k})^2}{2}+Q_m^{k}u_m^{k}-Q_{m-1}^{k}u_{m-1}^{k}\right)=\\ &=\frac{\mu}{2\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k+1}+\psi_{m-1/2}^{k+1}}\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k+1}+\psi_{m-3/2}^{k+1}}\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta q}\right)\right]+\\ &+\frac{\mu}{2\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k}+\psi_{m-1/2}^{k}}\frac{u_{m+1/2}^{k}-u_{m-1/2}^{k}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k}+\psi_{m-3/2}^{k}}\frac{u_{m-1/2}^{k}-u_{m-3/2}^{k}}{\Delta q}\right)\right]+\\ &+\frac{\mu}{\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k+1/2}+\psi_{m-1/2}^{k+1/2}}\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k+1/2}+\psi_{m-3/2}^{k+1/2}}\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta q}\right)\right]\end{aligned} \tag{17}$$

When using the finite difference method, not the initial partial differential equation is solved numerically, but some modified equation, called differential approximation of the

difference scheme [62,63]. The right-hand side of this approximation is the approximation error and is equal to the difference between the original partial differential equation and its finite-difference analogue. An analysis of the right-hand sides of differential approximations makes it possible to establish the predominant contribution to the error in approximating the higher derivatives and associated properties of difference schemes such as dissipation and dispersion. It is known that if the principal term in the expression for the approximation error contains derivatives of even order, then the predominant properties of the difference schemes will be dissipative, and if the derivatives of odd order – then will be dispersive.

Let us write down the differential approximation for the difference scheme (17). To obtain differential approximations, we use the standard procedure for expanding the grid functions in a neighborhood of the point $(m,m_{+1/2})$ in a Taylor series. Omitting simple but cumbersome transformations, we write the differential approximation in the final form.

$$\frac{Q}{\psi}\frac{\partial u}{\partial q}+\frac{1}{\psi}\frac{\partial}{\partial q}\left(\frac{u^2}{2}\right)-\frac{1}{\psi}\frac{\partial}{\partial q}\left(\frac{\mu}{\psi}\frac{\partial u}{\partial q}\right)=\frac{1}{\psi}\left(\alpha\frac{\partial^2 u}{\partial q^2}+\beta\frac{\partial^3 u}{\partial q^3}+\gamma\frac{\partial^4 u}{\partial q^4}+\delta\frac{\partial^3}{\partial q^3}\left(\frac{1}{\psi}\right)\right) \qquad (18)$$

The coefficients of the derivatives on the right-hand side of Eq. (18) α, β, γ, δ are expressed as follows

$$\alpha=-\frac{\Delta q^2}{32}\left(4\frac{\partial u}{\partial q}-\mu\frac{\partial^2}{\partial q^2}\left(\frac{1}{\psi}\right)\right),\quad \beta=\frac{\Delta q^2}{24}\left(\mu\frac{\partial}{\partial q}\left(\frac{1}{\psi}\right)-u+Q\right),\quad \gamma=\frac{\Delta q^2}{48}\frac{\mu}{\psi},\quad \delta=\mu\frac{\Delta q^2}{96}\frac{\partial u}{\partial q}$$

In the differential approximation (18), the most important role is played by the terms on the right-hand side of the second and third derivative equations, characterizing the dissipation and dispersion of the difference scheme, respectively. The coefficients α and β, standing respectively before the second and third derivatives, depend on the adaptation parameters. This means that the dissipation and dispersion of the difference schemes depend on the method of adaptation and can be changed in the necessary direction. The coefficient β explicitly depends on the fucntion Q, which allows, using the appropriate choice of Q to convert the coefficient β to zero. Thus, one can almost completely get rid of the internal dispersion of the difference scheme. The coefficient β vanishes if the function Q is set equal to:

$$Q=-\left(u-\frac{\partial}{\partial q}\left(\frac{\mu}{\psi}\right)\right) \qquad (19)$$

A similar analysis for a two-layer scheme was carried out in Refs. [35-36].

6.2 Modeling results

We consider the possibilities of reducing the error in the approximation of two and three-layer difference schemes by considering the numerical solution of the Burgers problem (1), (11), (12) using the dynamic adaptation method. For this, in the computational space $\Omega_{q,\tau}$ with variables (q,τ) we represent the Burgers equation (14) in a divergence form, and write the equation of the inverse transformation (15) in a modified, more convenient form

$$\frac{\partial(\psi u)}{\partial \tau} = -\frac{\partial(Q \cdot u)}{\partial q} - \frac{\partial}{\partial q}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial q}\frac{\mu}{\psi}\frac{\partial u}{\partial q}, \tag{20}$$

$$\frac{\partial \psi}{\partial \tau} = -\frac{\partial Q}{\partial q}, \qquad q_0 < q < q_R, \quad \tau > 0 \tag{21}$$

The equations (20), (21) are supplemented by the initial

$$u(q,0) = \sin(2\pi q) + 0.5\sin(\pi q) \qquad \psi(q,0) = 1$$

and boundary conditions:

$$u(q_0,\tau) = u(q_R,\tau) = 0 \qquad Q(q_0,\tau) = Q(q_R,\tau) = 0$$

The function Q was set in the form (19) $\qquad Q = -\left(u - \frac{\partial}{\partial q}\left(\frac{\mu}{\psi}\right)\right)$

6.3 Algorithm of numerical solution on a dynamic grid

Using a computational grid with integer and half-integer nodes, we write out a family of two-layer conservative difference schemes for the system of equations (20), (21). The functions x_m^k, u_m^k, Q_m^k are written in the integer nodes and the grid fucntions $\psi_{m+1/2}^k$ are written in the half-integer nodes $\left(q_{m+1/2}, \tau^k\right)$. The family of the two-layer difference schemes has the form:

$$(\psi u)_m^{k+1} = (\psi u)_m^k - \frac{\Delta\tau^k}{\Delta q}\left\{ (1-\sigma)\left[\frac{1}{2}\left(\frac{u_{m+1}^2}{2} - \frac{u_{m-1}^2}{2}\right) - \frac{\mu}{\psi_{m+1/2}}\frac{u_{m+1}-u_m}{\Delta q} + \frac{\mu}{\psi_{m-1/2}}\frac{u_m - u_{m-1}}{\Delta q} + \frac{(uQ)_{m+1} - (uQ)_{m-1}}{2}\right]^k + \right.$$
$$\left. + \sigma\left[\frac{1}{2}\left(\frac{u_{m+1}^2}{2} - \frac{u_{m-1}^2}{2}\right) - \frac{\mu}{\psi_{m+1/2}}\frac{u_{m+1}-u_m}{\Delta q} + \frac{\mu}{\psi_{m-1/2}}\frac{u_m - u_{m-1}}{\Delta q} + \frac{(uQ)_{m+1} - (uQ)_{m-1}}{2}\right]^{k+1} \right\} \tag{22}$$

$$\psi_{m+1/2}^{k+1} = \psi_{m+1/2}^k - \frac{\Delta\tau^k}{\Delta q}\left((1-\sigma)\left[Q_{m+1} - Q_m\right]^k + \sigma\left[Q_{m+1} - Q_m\right]^{k+1}\right) \tag{23}$$

$$Q_m = -\left[u_m - \frac{\mu}{\Delta x}\left(\frac{1}{\psi_{m+1/2}} - \frac{1}{\psi_{m-1/2}}\right)\right]$$

In the calculations, the Crank-Nicolson scheme (σ = 0.5) was used with the second order of approximation O($\Delta\tau^2 + \Delta q^2$). Since the dynamic adaptation mechanism is formulated at the differential level, the main differences between the computational algorithm in the variables

(q,τ) are associated with the appearance of an additional equation (21). A system of two-layer difference schemes (22), (23) was solved by separate sweeps with internal and external iterations.

The algorithm for the numerical solution of an implicit three-layer scheme, as in variables (x,t), consists of three stages. First, a system of nonlinear algebraic equations is solved in the first half-step in time, from which the conservative variables $u_{m-1/2}^{j+1/2}$ are found.

$$\begin{aligned}
&\frac{\psi_{m-1/2}^{k+1/2}u_{m-1/2}^{k+1/2}-\psi_{m-1/2}^{k}u_{m-1/2}^{k}}{\Delta\tau/2}+\frac{1}{2}\frac{1}{\Delta q}\left(\frac{(u_m^{k+1})^2}{2}-\frac{(u_{m-1}^{k+1})^2}{2}+Q_m^{k+1}u_m^{k+1}-Q_{m-1}^{k+1}u_{m-1}^{k+1}\right)+\\
&+\frac{1}{2}\frac{1}{\Delta q}\left(\frac{(u_m^{k})^2}{2}-\frac{(u_{m-1}^{k})^2}{2}+Q_m^{k}u_m^{k}-Q_{m-1}^{k}u_{m-1}^{k}\right)=\\
&=\frac{1}{2}\frac{\mu}{\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k+1/2}+\psi_{m-1/2}^{k+1/2}}\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k+1/2}+\psi_{m-3/2}^{k+1/2}}\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta q}\right)\right]+\\
&+\frac{1}{2}\frac{\mu}{\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k}+\psi_{m-1/2}^{k}}\frac{u_{m+1/2}^{k}-u_{m-1/2}^{k}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k}+\psi_{m-3/2}^{k}}\frac{u_{m-1/2}^{k}-u_{m-3/2}^{k}}{\Delta q}\right)\right]
\end{aligned} \tag{24}$$

At the secodn stage – extrapolation of stream variables within space-time cells is performed

$$u_m^{k+1}=\begin{cases}2u_{m-1/2}^{k+1/2}-u_{m-1}^{k}, & for \quad \left(u_{m-1/2}^{k+1/2}-Q_{m-1/2}^{k+1/2}\right)>0;\\ u_{m-1/2}^{k+1/2}+u_{m+1/2}^{k+1/2}-u_m^{k}, & for \quad \left(u_{m-1/2}^{k+1/2}-Q_{m-1/2}^{k+1/2}\right)=0;\\ 2u_{m+1/2}^{k+1/2}-u_{m+1}^{k}, & for \quad \left(u_{m-1/2}^{k+1/2}-Q_{m-1/2}^{k+1/2}\right)<0;\end{cases} \tag{25}$$

At the third stage, the system of difference equations is solved at the second half-step so the conservative variables $u_{m-1/2}^{k+1}$ are found at the new time layer

$$\begin{aligned}
&\frac{\psi_{m-1/2}^{k+1}u_{m-1/2}^{k+1}-\psi_{m-1/2}^{k+1/2}u_{m-1/2}^{k+1/2}}{\Delta\tau/2}+\frac{1}{2}\frac{1}{\Delta q}\left(\frac{(u_m^{k+1})^2}{2}-\frac{(u_{m-1}^{k+1})^2}{2}+Q_m^{k+1}u_m^{k+1}-Q_{m-1}^{k+1}u_{m-1}^{k+1}\right)+\\
&+\frac{1}{2}\frac{1}{\Delta q}\left(\frac{(u_m^{k})^2}{2}-\frac{(u_{m-1}^{k})^2}{2}+Q_m^{k}u_m^{k}-Q_{m-1}^{k}u_{m-1}^{k}\right)=\\
&=\frac{1}{2}\frac{\mu}{\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k+1}+\psi_{m-1/2}^{k+1}}\frac{u_{m+1/2}^{k+1}-u_{m-1/2}^{k+1}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k+1}+\psi_{m-3/2}^{k+1}}\frac{u_{m-1/2}^{k+1}-u_{m-3/2}^{k+1}}{\Delta q}\right)\right]+\\
&+\frac{1}{2}\frac{\mu}{\Delta q}\left[\left(\frac{2}{\psi_{m+1/2}^{k+1/2}+\psi_{m-1/2}^{k+1/2}}\frac{u_{m+1/2}^{k+1/2}-u_{m-1/2}^{k+1/2}}{\Delta q}\right)-\left(\frac{2}{\psi_{m-1/2}^{k+1/2}+\psi_{m-3/2}^{k+1/2}}\frac{u_{m-1/2}^{k+1/2}-u_{m-3/2}^{k+1/2}}{\Delta q}\right)\right]
\end{aligned} \tag{26}$$

The difference schemes of the first (24) and third (26) stages were solved together with the scheme (21). The principal point of the computational algorithm is the elimination from the solution of the procedure of non-linear flux correction (monotonization), since it turns out to be excessive.

6.4 Analysis of the computaion results

The numerical solution of problem (20) - (21) in the perameter range $\mu \in \left(10^{-3} \div 10^{-6}\right)$ was carried out by means of two and three-layer difference schemes (22), (23) and (24) - (26). All calculations were carried out on adaptive grids with the same number of nodes. To achive the same precision as with the grids with fixed nodes, the number of nodes for the adaptive grid N = 25 turned out to be by 2 orders lower. Fig. 8,9 show the spatial profiles of the grid functions $u(x)$ and $\psi(x)$ at 4 moments of time for $\mu = 10^{-4}$. The results of calculations using the two-layer (22), (23) and three-layer (24)-(26) schemes showed a good match between each other and the exact solution. The profiles of the function $u(x)$ are completely free from the parasitic oscillations. In this case, the three-layer scheme (24) - (26) does not contain a flux correction procedure. As in the case of using the two-layer scheme, the improvement of the quality of the solution in the three-layer scheme is achieved due to the controlled distribution of the grid nodes, the motion of which is completely coordinated with the sought solution.

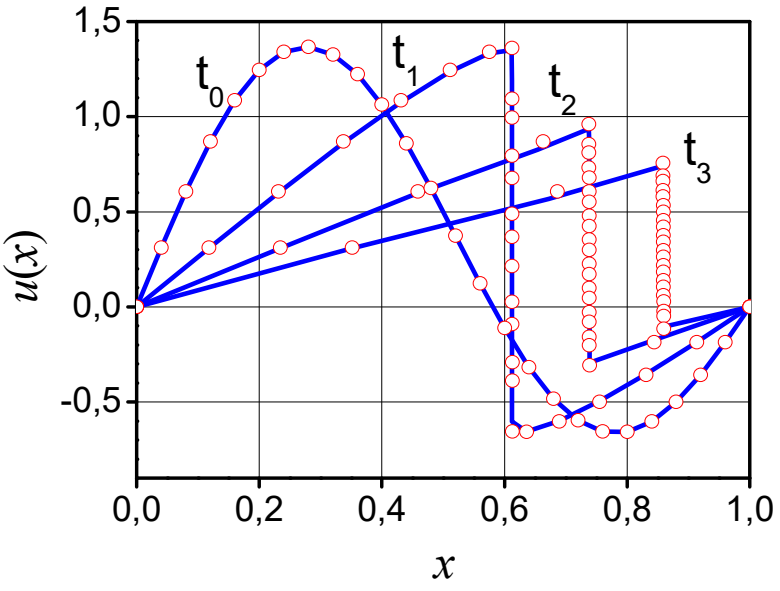

Fig. 8. Spatial profile of the function *u(x)* at different moments.

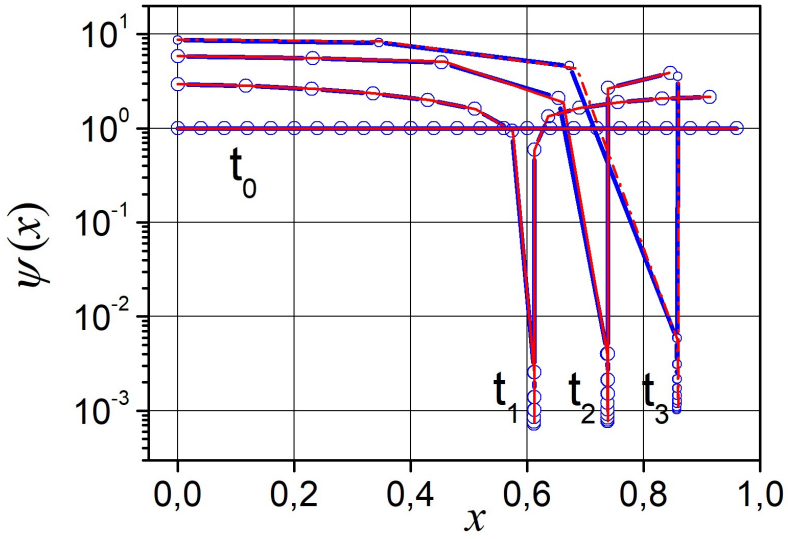

Fig. 9. Spatial profiles of the function *ψ(x)* at different moments.

The dynamics of distribution of the grid nodes in the physical space $\Omega_{x,t}$ with variables (x,t) is characterized by the function $\psi(x)$, Fig. 9. The function $\psi(x)$ representing the ratio $\psi(x) \approx \Delta x / \Delta q$ characterizes the dimensionless spatial step of the grid in the space $\Omega_{x,t}$ since Δq does not change with time. The function $\psi(x)$ shows how much the spatial grid step $\Delta x(t)$ changes at each moment of time.

The spatial profiles of $u(x)$ and $\psi(x)$ indicate a smooth concentration of the grid nodes in the region of the front of the function, which corresponds to a decrease in the grid spacing by 3 orders of magnitude, Fig. 9, with a simultaneous increase in the grid spacing by 2-9 times in the region of a slow change in the solution.

Thus, due to full conformity with the sought solution, dynamic adaptation turned out to be a more subtle and flexible mechanism for reducing the error of approximation of difference schemes in comparison with the method of nonlinear correction of fluxes.

7 CONCLUSION

- The families of two-layer and three-layer difference schemes of the second order for the complete burgers equation in fixed cartesian and arbitrary non-stationary coordinate systems were constructed.
- Modeling with the subsequent analysis of its results has shown that in the cartesian coordinate system the quality of the numerical solution essentially depends on the quality of the finite-difference approximation used for the initial equation.
- The main drawback of three-layer difference schemes is the presence in the region of large gradients of a difficultly removable deviation of the numerical solution from the exact one, which is caused by the process of forced monotonization of the solution. This circumstance stimulates the search for other ways of reducing the error of approximation.

- The use of non-stationary coordinate systems makes it possible to change the approximation error in the course of the solution by controlling the motion of the grid nodes, in contrast to stationary coordinate systems in which the approximation error is determined by the original structure of the difference scheme. The application of an arbitrary non-stationary coordinate system made it possible to create a universal dynamic adaptation method for a wide class of problems in mathematical physics in which the distribution of nodes is dependent and controlled by the sought solution. This makes it possible to automatically adjust the calculated grid in such a way that the approximation error is minimal practically regardless of the quality of the original difference scheme. The numerical solution of the nonlinear burgers equation with the help of two and three-layer difference schemes on a dynamically adapting grid showed virtually complete coincidence of the calculations among themselves, good agreement with the exact solution with complete absence of oscillations in the solution. The computational grid contained the number of nodes (N = 25) by two orders of magnitude smaller than the grid with fixed nodes.
- Dynamic adaptation of grids is an independent, flexible and the most accurate way of reducing the approximation error, in particular in the problems of convection-diffusion with the dominant convection mechanism.

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