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*Rapport
de recherche*

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Reminiscences about numerical schemes

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Abstract: This preprint appeared firstly in Russian in 1997. Some truncated versions of this preprint were published in English and French, here a fully translated version is presented. The translation in English was done by O. V. Feodoritova and V. Deledicque to whom I express my gratitude.

Key-words: Godunov's Scheme, hyperbolic systems of conservation laws.

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‡ This preprint is a talk that was given at the International Symposium entitled "Godunov's Method in Gas Dynamics", Michigan University (USA), May 1997.

Reminiscences about numerical schemes

Résumé : Une version, écrite en russe, est apparue la première fois en 1997. D'autres versions (anglaise et française) ont été publiées mais sous forme abrégée. On présente ici une traduction complète du document original en anglais, traduction effectuée par O. V. Feodoritova et V. Deledicque, envers lesquels j'exprime ici toute ma gratitude.

Mots-clés : Schéma de Godunov, systèmes hyperboliques de lois de conservation.

Introduction

In the present paper I will describe how the first variant of the "Godunov's scheme" has been elaborated in 1953-1954 and tell about all modifications realized by myself (until 1969) and the group of scientists from the Institute of Applied Mathematics in Moscow (which has become the M.V.Keldysh Institute of Applied Mathematics).

At the time these modifications (see Sections 2,3) were carried out, other algorithms were developed, in particular second order schemes for gas dynamics problems with a small number of strong and weak discontinuities [1-3]. We performed many calculations based on the first codes written by V. V. Lucikovich. More complicated problems resulted in an elaboration of very artful approaches to divide the whole computational domain into sub-domains which have been developed by A.V.Zabrodin. This procedure resulted in the necessity to develop algorithms of grid construction.

In 1961-1968 G. P. Prokopov and I carried out approaches to the construction of moving grids which were used in serial calculations by A. V. Zabrodin, G. N. Novozhilova and G. B. Alalikin (see [4-6]). The problems appearing in the grid construction forced us to solve elliptical systems (see [7-8]). The methods elaborated here, have later been employed in elliptical spectral problems and have been presented in my papers on numerical linear algebra (see [9,10]). The number of interesting observations made during the analysis of my calculations gave many discussions at the Moscow University and, after 1969 – at the Novosibirsk University. As a result of such discussions the criterion of spectral dichotomy [11,12] has been developed and high-precision algorithms to calculate singular vectors have been constructed (see [11,13]). It is difficult to imagine that the reason of such investigations has been the elaboration of approaches to the gas dynamics calculus and numerical grid constructions.

During my studies at Moscow University I learned the differential equations theory in seminars of I. M. Gelfand and I. G. Petrovskii. The latter focused my attention on gas dynamics problems and proposed to me to use stationarization methods to study transitional flows (with sub- and supersonic regions). My qualification work was devoted to the stationarization of a flow inside a nozzle (however, only in subsonic regime and with artificially added time derivatives introduced in Chaplygin's equation). Petrovskii's idea about stationarization in practical form was published in 1961 (see [6]). The technical statement was presented in the qualification work of G. P. Prokopov performed under my supervision. The coding was made by G. N. Novozhilova.

The elaboration of numerical schemes was carried out at the same time with attempts to have a better understanding of the notion of generalized solutions to quasi-linear systems of equations. As a rule, the hypothesis about possible definitions and properties of the generalized solutions were preceded to the construction of numerical schemes, which used these properties. At the same time, I tried to prove the formulated hypothesis. To my deep disappointment, these attempts had no success. On the contrary, they often led to contradictory examples. But, at the same time, a numerical scheme, more precisely its modification, based on using the Euler coordinates, moving grids and tracking methods for strong and weak discontinuous, was used in customary calculations.

1 How the scheme has been elaborated

In autumn 1953 M. V. Keldysh and I. M. Gelfand proposed me to elaborate a variant of a method suggested by J. Von Neumann and R. D. Richtmyer. It consisted in the introduction of artificial viscosity in the gas dynamics equations. The goal was to finish the algorithm for serial engineering calculations by the spring of 1954. By this time, the first electronic numerical device "Strela" had to be delivered at our Institute.

I knew that one variant of the required algorithm in our Institute had been prepared by A. I. Zhukov. I had the opportunity to study it and the goal was to modify this algorithm

or to suggest a new variant. From the point of view of the administration of our Institute it was necessary to continue the study in this direction to be able to solve efficiently this problem to a fixed date.

The method of A. I. Zhukov exactly coincided with the scheme published by P. D. Lax one year later [14]. The paper I received from A. I. Zhukov contained some ideas and hypotheses on which the numerical scheme was based. Some of the hypotheses were erroneous but during my first reading of the paper I was confident in them and decided to rely on these hypotheses in my work.

The principal difference between Zhukov's method and the approach by J. Von Neumann and Richtmyer lies in the use or not of the artificial viscosity. A. I. Zhukov understood during his experiments that smearing of shock waves was made automatically because of discrepancy between approximate and exact differential gas dynamics equations. A. I. Zhukov explained this discrepancy by analyzing the truncation terms of the difference scheme, which present *numerical viscosity*, and formulated the idea of *the first differential approximation*.

He began to use the second order difference schemes but faced with strong oscillations near the shock wave front. To explain this fact he used exact solutions based on Airy functions of linearized equations in which numerical viscosity was introduced to model truncation terms of the numerical scheme. The experiments resulted in the conclusion that the second order schemes had to be avoided, and A. I. Zhukov concentrated on the development of the first schemes for the simplest quasi-linear Burgers equation and the gas dynamics equations in the Lagrangian coordinates. The whole attention was concentrated on the investigation of numerical solutions of problems with a steadily moving shock front. When the first differential approximation was used, the problem was reduced to the solution of the ordinary differential equations which could be compared with numerical solutions. Based on these comparisons A. I. Zhukov formulated a necessary condition which any difference scheme should satisfy. This condition means that the first differential approximation should have the form of conservation laws, however it was formulated as a hypothesis of a necessary and sufficient condition.

I did not doubt in that hypothesis and put it in the cornerstone of my attempts to build a scheme without oscillations but with second order accuracy. To reach this goal I began to compare different second order schemes which are not conservative but they are conservative at the first order. The comparison of different variants was based on the same solutions which were important for a whole set of typical problems. As a result a rather satisfactory variant was chosen. Three months of intensive work were spent for such a choice. N. M. Zueva helped to perform calculus, and numerical experiments were performed by V. V. Paleichik and two of her students who studied technology of calculation based on mechanical adding machine "Mercedes". M. V. Keldysh and I. M. Gelfand were interested in these investigations; they listened to reports about the current state of this work biweekly.

The next stage of the investigations was to prove the efficiency of the scheme based on various numerical experiments with different spatial steps and different solutions. But already during investigation of the dependence of the solution on the spatial step we faced with the situation that completely crossed out all results of our three-month work.

To clarify the difficulties we have faced I have to tell about one hypothesis from Zhukov's report. He compared the solution of a problem about steadily moving shock waves by using the first differential approximation with the real profile obtained from the numerical calculations. They were different and he supposed that this difference would be decreased if the spatial step tends to zero.

I decided to check this hypothesis and asked V. V. Paleichik to make corresponding calculations. One set of calculations with one step size was made by the first student, and the calculations with one-half of that step by another. Rapidly, in five-ten minutes V. V. Paleichik reported me about senseless of the proposed experiment. The results of both experiments were absolutely the same, and obviously a different result was not possible because spatial step itself did not play any role in calculations. Only the relation between

time and spatial steps took part in the experiments and it was chosen constant to keep Courant's number constant. So, finite-difference profiles were not modified in the process of step decreasing and did not converge to the dimensionless profile obtained for the first differential approximation. At the same time, the comparison of the velocity of the exact and finite-difference shock fronts demonstrated no significant difference ($\approx 3 - 4\%$), but this difference did not decrease during steps reduction.

Obviously, this situation put me under stress and forced me to change my previous point of view.

Firstly, it was obvious that the numerical scheme should guarantee the correct velocity of a steadily moving shock wave and correct values on both sides of the front *even if the step size equals to 1*. The hope, that the accuracy in calculation would be high if the step was small enough, disappeared.

The conclusion was to use exact conservation laws without simplifications related to the use of conservation laws obtained from the first differential approximation. For this, the approximation of the equations

$$\begin{aligned}\frac{\partial u}{\partial t} + \frac{\partial p(v)}{\partial x} &= 0, \\ \frac{\partial v}{\partial t} - \frac{\partial u}{\partial x} &= 0,\end{aligned}$$

should be done to provide the following conservative form of difference equations

$$\begin{aligned}\frac{u_n^{m+1} - u_n^m}{\Delta t} + \frac{P_{n+\frac{1}{2}}^m - P_{n-\frac{1}{2}}^m}{\Delta x} &= 0, \\ \frac{v_n^{m+1} - v_n^m}{\Delta t} - \frac{U_{n+\frac{1}{2}}^m - U_{n-\frac{1}{2}}^m}{\Delta x} &= 0.\end{aligned}$$

To describe the velocity field one should use both u_n^m and $U_{n+\frac{1}{2}}^m$. Similarly, the specific volume v and pressure $p(v)$ related to it are approximated by both v_n^m and $P_{n+\frac{1}{2}}^m$ respectively. The different formulas connecting the lower and upper case letters result in the different schemes. The resulting scheme should provide the smoothness of a numerical profile. Based on this scheme and numerical conservation laws one can conclude that velocity of the wave is correct and values on the right and left sides of the shock are connected by the known Hugoniot relations.

To construct a scheme I decided at first to obtain a smooth front in the limit case of weak waves, i.e. in the case of acoustic equations, which can be considered as the gas-dynamics equations with the simplest equation of state $p(v) = -a^2 v$ ($a^2 = \text{const.} > 0$). In this case, the shock waves are transformed into the discontinuities of the Riemann invariants $u \pm a v$, and the equations are reduced to a canonical form

$$\frac{\partial(u \pm a v)}{\partial t} \mp a \frac{\partial(u \pm a v)}{\partial x} = 0.$$

I decided to choose numerical schemes which allow (at least in this simplest case $p(v) = -a^2 v$, $a = \text{const.}$) the reduction of these equations to independent equations for the Riemann invariants $u \pm a v$. I used the simplest scheme conserving the monotonicity of the Riemann invariants which was known and widely used at that time. The monotonicity guaranteed a required smoothness. At that time I did not have another criterion and there was no more time for proposing something else. "Strela" was already being installed in our Institute. At that time I could show for the linear case that only the first order schemes conserve the monotonicity. I decided not to provide further efforts in order to construct second order schemes.

The chosen scheme in the simplest case had the following form :

$$\begin{aligned} \frac{u_n^{m+1} - u_n^m}{\tau} - a^2 \frac{v_{n+1}^m - v_{n-1}^m}{2h} - a \frac{u_{n+1}^m - 2u_n^m + u_{n-1}^m}{2h} &= 0, \\ \frac{v_n^{m+1} - v_n^m}{\tau} - \frac{u_{n+1}^m - u_{n-1}^m}{2h} - a \frac{v_{n+1}^m - 2v_n^m + v_{n-1}^m}{2h} &= 0, \end{aligned}$$

and transformed into a finite-difference conservation laws after introduction of the following notations

$$\begin{aligned} P_{n+\frac{1}{2}}^m &= -a^2 \frac{v_{n+1}^m + v_n^m}{2} + a \frac{u_{n+1}^m - u_n^m}{2} = \frac{p(v_{n+1}^m) + p(v_n^m)}{2} + a \frac{u_{n+1}^m - u_n^m}{2}, \\ U_{n+\frac{1}{2}}^m &= \frac{u_{n+1}^m + u_n^m}{2} + a \frac{v_{n+1}^m - v_n^m}{2} = \frac{u_{n+1}^m + u_{n-1}^m}{2} - \frac{p(v_{n+1}^m) - p(v_n^m)}{2a}. \end{aligned}$$

It was decided to use the scheme in a general nonlinear case, but the constant a in formulas $P_{n+\frac{1}{2}}^m, U_{n+\frac{1}{2}}^m$ had to be replaced by some, generally speaking, non-constant values $a_{n+\frac{1}{2}}^m$. The first variant to calculate $a_{n+\frac{1}{2}}^m$ was the following

$$\begin{aligned} a_{n+\frac{1}{2}}^m &= \sqrt{-p'(v_n^m + v_{n+1}^m)}, \\ a_{n+1}^m &= \frac{1}{2} \left(\sqrt{-p'(v_n^m)} + \sqrt{-p'(v_{n+1}^m)} \right), \\ a_{n+1}^m &= \sqrt[4]{p'(v_n^m)p'(v_{n+1}^m)}. \end{aligned}$$

These formulas were tested in the numerical experiments during which the monotonicity of the shock profile was checked. The initial data for the shock were chosen as constant values on the right and left sides of the discontinuity. These constant values were connected by Hugoniot relations.

During these experiments I began using other formulas for $a_{n+\frac{1}{2}}^m$. In particular, I wanted to conserve monotonicity at the first step and I could construct some interpolation formula for $a_{n+\frac{1}{2}}^m$ which gave the most acceptable results.

Here I should add some precisions to my story to correct the simplifications I introduced. We soon began the above described experiments not with the simplest gas dynamics equations we used before but with the system of three equations

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial p(v, E)}{\partial x} &= 0, \\ \frac{\partial V}{\partial t} - \frac{\partial u}{\partial x} &= 0, \\ \frac{\partial}{\partial t} \left(E + \frac{u^2}{2} \right) + \frac{\partial (p u)}{\partial x} &= 0, \end{aligned}$$

with the following form of numerical conservation laws

$$\begin{aligned} \frac{u_n^{m+1} - u_n^m}{\Delta t} + \frac{P_{n+\frac{1}{2}}^m - P_{n-\frac{1}{2}}^m}{\Delta x} &= 0, \\ \frac{v_n^{m+1} - v_n^m}{\Delta t} - \frac{U_{n+\frac{1}{2}}^m - U_{n-\frac{1}{2}}^m}{\Delta x} &= 0, \\ \frac{\left(E + \frac{u^2}{2} \right)_n^{m+1} - \left(E + \frac{u^2}{2} \right)_n^m}{\Delta t} + \frac{P_{n+\frac{1}{2}}^m U_{n+\frac{1}{2}}^m - P_{n-\frac{1}{2}}^m U_{n-\frac{1}{2}}^m}{\Delta x} &= 0. \end{aligned}$$

A selection of the interpolation formulas for $a_{n+\frac{1}{2}}^m$ became in this case a selection of variants to calculate $P_{n+\frac{1}{2}}^m, U_{n+\frac{1}{2}}^m$ as a function of $u_n^m, v_n^m, E_n^m, u_{n+1}^m, v_{n+1}^m, E_{n+1}^m$.

The adequate variant has been found after 2-3 weeks. It is important to remark that in the chosen formulas the role of $a_{n+1/2}^m$ played the expressions

$$\sqrt{\frac{(\gamma + 1)P_{n+1/2} + (\gamma - 1)p_n}{v_n}}$$

which depended on the quantity $P_{n+1/2}$ (in these experiments the equation of state $E = (pv)/(\gamma - 1)$ was used). It occurred to me that I saw such expressions somewhere in the literature.

Not long before to that the book of L. D. Landau and E. M. Lifshitz "The Mechanics of Continuous Media" was published. In this book these quantities took part in formulas which described the solution of the Riemann problem. I had to modify slightly my interpolation formulas to obtain the final form of my scheme. These modifications were significant only in the case of strong rarefaction waves. It happened in March 1954. At the end of March, V. V. Lucikovich was included in our group to write a code according to technical tasks that we composed by taking into account useful recommendations of K. A. Semendjaev. At the end of April I was on holidays for two weeks, and on the 5th May we began our experimental and applied calculations.

On the 4th of November 1954 I defended my PhD thesis containing the description of the suggested scheme. But this work was published only in 1959. Just before, I tried to publish the work in some journals without success. The journal "Applied Mathematics and Mechanics" refused to publish it because it was purely mathematical and without any relation to mechanics. In one mathematical journal (I do not remember which one) the refusal was motivated with the opposite statement. After that I. G. Petrovskii as a member of the editorial group helped to publish it in the journal "Matematicheskii Sbornik" (see [15]).

I read the paper by P. D. Lax [14] only after my PhD thesis defense. The scheme described in this work coincided with Zhukov's scheme but without questionable hypotheses which were in Zhukov's report and whose analysis helped me to construct my scheme. If I had received this paper one year earlier, the "Godunov's scheme" would never have been constructed.

2 Problems of approximation and effective accuracy

Indeed, the work on modifications of the scheme invented in 1954, was actively pursued. Consumers were very suspicious toward my scheme.

In our Institute, more precisely, in Steklov's Institute, from which Keldysh's Institute was separated in 1953, the basic hydrodynamic calculations were organized by K. A. Semendjaev much before I came. They were made with the help of the mechanical adding machine "Mercedes" using the method of characteristics by a large group of colleagues. The algorithm was thoroughly thought over by K. A. Semendjaev and A. I. Zhukov. The basic attention was payed to the table of results and the reduction of intermediate records. This reduction was provided with memory cells of the "Mercedes". All results were presented in graphical form and checked very carefully.

The technique of the calculations was absolutely automatic. My female colleagues worked on machines as pianists and simultaneously discussed their household and other typical problems of female interest. They mocked especially young researchers among whom I was. We were named by the contemptuous word "that science". They supposed we built pseudo-scientific theories, useless to overcome difficulties which only led to the delay of calculations. One should remark, their salary depended on the calculation volume which was defined by the number of table rows without mistakes.

The graphical presentation of results on a graph paper had a very high quality, and contained a visual plot of velocity, pressure and density fields, and also the trajectories of

contact discontinuities and characteristics giving the possibility to follow the domain of influence of the initial data.

Our customers - physicists and engineers – had a habit to a perfect form of the information obtained and it was a reason of their displeasure toward the first calculation results based on numerical schemes. Now it is well-known that the numerical calculations of the discontinuous gas dynamics solutions present a "numerical" micro-structure which looks like errors providing a caricatural picture of the real flow. The comparison of computer and "hand-made" calculations resulted in the opinion that the code had errors or that the initial data were erroneous. We had to check carefully all situations, we had to explain the results and to modify either the results or the calculation scheme.

I will describe now two such examples, the most interesting from my point of view.

During calculations based on my scheme of strong isentropic rarefaction waves one could observe a significant growth of the entropy which was the source of distrust toward the numerical results. One noticed a substantial reduction of such effect only after 3-4 years (in 1957-1958) when we studied 2-D problems. Such problems, as a rule, do not have a simple formulation in the Lagrangian coordinates and we had to use the Eulerian description. Simultaneously, numerical grids became complicated, they became moving ones. The main idea - to use the exact solution of the Riemann problem as an element of a numerical scheme - has been applicable in 2-D problems also, but not in a transparent way. The first test calculations of 1-D problems earlier computed were repeated using new 2-D codes. We were very surprised by the fact that 2-D codes based on the Eulerian coordinates resulted in essentially less parasitic increasing of the entropy in the rarefaction waves.

The reason of the effect is that the Lagrangian coordinates (even in the simplest 1-D case) are unfit to the formulation of the generalized solutions of the gas dynamics equations. These equations admit the formation of vacuum regions which are treated in the Lagrangian coordinates by singularities of the delta function type. Usually such singularities are not supposed to be present, and they are modelled very badly numerically. The analysis of the results showed that even a sufficient decreasing of the step size in Lagrangian coordinate in a strong rarefaction zone does not result in a noticeable distance reduction between Eulerian coordinates of neighboring nodes. I used this fact in 1961 in the theoretical work [16] to prove that my scheme approximates (if the Eulerian coordinates are used) the gas dynamics equations in a sense of conservation laws (1-D case). At the beginning of this work I hoped to prove a convergence to the exact solution but I failed to that. Even the order of approximation appeared to be different from one, it was equal to $2/3$. Remember that, formally, my scheme has the first order of approximation based on the first differential approximation. I should remark that indeed the order of approximation is probably higher than $2/3$. Apparently, based on estimates of the variations of solution suggested by J. Glimm [17] one can prove that this order is equal to one. Unfortunately I did not investigate this issue in details. However at the end of the 50th I was interested basically in the accuracy of the approximated solutions, and not in the problem of approximation of equations (i.e. what power of the spatial step evaluates the error - the difference between the calculation result and the exact solution). The obtained estimates for approximation played a preliminary role for theoretical investigation which I could not finish. Despite of it, in 1957-1958 V.S. Ryabenkii and I carried out an experimental study of the convergence of approximate solutions calculated with my scheme to the exact solution. These observations about calculation results allowed me to conclude that the convergence had to be considered as *weak* and not *strong* to exclude the influence of significant deviations in one-three nodes. As a rule, the occurring of these deviations is related to the interaction of two shock waves or reflection of a shock wave from a contact discontinuity.

During our discussions, V. S. Ryabenkii suggested an approach which permitted us a reduction of the study of weak convergence to the study of strong convergence *in 1-D problems*. For this, one needs to compare not quantities controlled by conservation laws but integrals (or even multiply integral) of these quantities with respect of spatial coordinate. We supposed to demonstrate the first order of weak convergence, i.e. the order correspond-

ing to a formal order of approximation. We were very surprised to see that the observed effective convergence order was less than 1 in experiments with centered expansion waves or large gradients in smooth domains restricted by strong discontinuities.

At that time we were very busy and had no motivation to prepare a detailed paper, especially because the conclusions were unpleasant to us (to me at least) and did not correspond to our expectations. I only made a brief presentation at a scientific conference at the Moscow University. From my point of view, nobody put attention on this presentation except N. S. Bachvalov who began the theoretical study of the convergence rate for the solutions for the Burgers equation as $\varepsilon \rightarrow 0$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \varepsilon \frac{\partial^2 u}{\partial x^2},$$

and obtained the estimate of the error $\varepsilon \ln |\varepsilon|$. At the same time, all my attempts to attract attention of researchers and engineers to these effects had no success.

My colleagues A. V. Zabrodin, K. A. Bagrinovskii, G. B. Alalikin and I were involved at that time in preparing 2-D calculations. That is the reason why the question if the first order scheme has the first order convergence rate, or, more precisely, what is this order, was not understood.

I know that later B. van Leer, P. Woodward, P. Collela, P.D. Lax, A. Harten and many others (see for instance [18-21]) suggested to construct efficient numerical schemes with order of approximation higher than one. At that time I had already left Keldysh Institute in Moscow and moved to Novosibirsk. Here I was involved in other problems. Among these issues the basic place was devoted to problems which arose during my work in Moscow and they required deep theoretical investigations. They were, in particular, issues concerning an accurate mathematical formulation of the conservation laws and thermodynamical identities, energy integrals for the hyperbolic equations, the mathematically correct formulation of the elasticity theory, and the statement of problems in numerical methods of linear algebra. I had already mentioned that this latter issue appeared from attempts to construct 2-D numerical schemes. The investigation of these various and interesting problems (see for instance [22,23]) did not allow me to continue the study of numerical methods and a deep understanding of modern numerical schemes for the gas dynamics equations, some of which named "*second order Godunov's schemes*". I claim I cannot be considered as the author of them. Maybe, their authors were inspired by my suggestion about using the exact solutions of elementary problems to construct a numerical scheme. It is my pleasure to thank them for the attention they payed to me.

Recently, two years ago, I learned that V. V. Ostapenko (Lavrentiev Institute of Hydrodynamics SB RAS, Novosibirsk) studied actively the problem of an effective accuracy of numerical schemes in hydrodynamics based on asymptotic expansions. Instead of performing cumbersome analytical calculations, I advised him to make the experimental investigations of the scheme we constructed together with V. S. Ryabenkii in 1957-1958. I hoped he would repeat our experiments and they would be described at last in details. But V. V. Ostapenko concentrated on the investigation of a more modern Lax-Harten scheme [19,21]. This scheme also demonstrated a mismatch between the formal order of approximation and the effective order of accuracy (order of convergence). At the same time, from the experimental results of V. V. Ostapenko it apparently followed that the accuracy of the Lax-Harten scheme in the sense of weak convergence on discontinuous solutions is not less than the first order, i.e. the accuracy is higher than for my original scheme.

I think, it is very interesting to carry out massive experimental investigations of precision for all principal numerical methods. Especially interesting would be such a study for 2-D and 3-D problems which require the elaboration of the corresponding experimental techniques.

One should remark the active work of K. A. Semendjaev to transform my scheme into a final computer code. His experience was very useful for our success.

3 2-D problems and moving grids

Despite the fact that the work on the 1-D approach has been continued I started thinking on a 2-D variant of my algorithm. The attempts to solve gas dynamics problems were done in Steklov's Institute and later in our Institute by K. I. Babenko and I. M. Gelfand. Appearing difficulties were discussed on seminars where M. V. Keldysh took part. In particular during these works and accompanying discussions the numerical schemes – explicit in one spatial variable and implicit in the other one ("sausages") – appeared. Also the first variant of the matrix double-sweep method that was suggested by M. V. Keldysh and investigated by K. I. Babenko and N. N. Chentsov appeared. There were a lot of discussions after the Locutsievskii's report based on the Rayleigh's book "Theory of Sound" chapter devoted to the instability of a contact discontinuity. Indeed, the contact discontinuity evolves in time according to the law described by differential equations for which the Cauchy problem is not well posed in Hadamard's sense (and not only its solutions are instable). The non well-posedness is characterized by the following fact – the short waves increase their amplitude very fast, the smaller the wave length is, the faster it is. The instability is a similar phenomenon, but in this case the characteristic time, during which the amplitude of the wave is increased, is bounded for all wave lengths. It was thought that processes described by the equations which are non well-posed in Hadamard's sense could not be computed numerically because numerical schemes should be unstable. We discussed some regularizations of the boundary conditions on the contact discontinuity. However I cannot remember if any realistic variant of such a regularization was developed.

Impressed by these discussions I got into a panic about the problems where contact discontinuities appeared. At that time there was a large interest in the problems that could be considered as near 1-D, i.e. the problems with slightly curved shocks and sound fronts and almost plane contact discontinuities. It occurred to me that for these problems a simple generalization of my scheme could be applied, and I started developing such generalization. My solution was supported by M. V. Keldysh and I. M. Gelfand. K. A. Bagrinovskii and G. B. Alalykin took part in the development of the first variant of algorithm. Later, A. V. Zabrodin joined us. The codes were again developed by V. V. Lucikovich and G. N. Novozhilova. It is interesting to note that, when the 2-D computer code has been written, the problems became more complex due to increasing demands of engineering interests. These complications led to modifications of the code and of the elements of the computational method. Busy with the computer code we forgot about the main danger – non well-posedness of the contact discontinuity. As far as I remember this non well-posedness did never appear.

I cannot understand why we did not meet this non well-posedness. Apparently, finite-difference equations used for the calculation of the boundary trajectories provide some forced regularization. If it is really so, one should be anxious about the following. The mechanism of this regularization is unknown, and hence we are not able to guarantee that it does not produce some undesirable effects.

From my point of view, *the detailed analysis of the algorithms used for the calculation of contact discontinuities is still an actual problem*. In this case, we can expect that some new effects will be discovered.

One should note that calculations with moving grids, in which the tracked shock wave induces the displacement of points in 2-D and 3-D grids, has not been studied carefully, neither theoretically nor experimentally. The feedback of such point displacements has not been investigated. And it is not clear what kind of effects this feedback produces.

When we implemented the 2-D approach based on the solutions of the Riemann problem with arbitrary initial conditions, the first question concerned the construction of such solutions. In the 2-D case the rectangular grid cells can neighbor not only on each other but also on the nodes where four cells meet. If one constructs a 2-D scheme analogously to the 1-D, one should have analytic solutions of hydrodynamical equations with four discontinuities of initial data at one point. We did not have such solutions, even now they do not

exist, at least for general initial data. We had the audacity to suggest to use only classical solutions of the Riemann problem combined from the plane waves and describing initial Riemann problem placed on the edges of the neighboring cells. We ignored interaction of four cells having a common node. Implementing this approach we abandoned a clear physical interpretation on which the construction of the 1-D scheme was based. Obviously, there were a lot of discussions about the suggestion mentioned above. As a result we decided to perform the investigation with the help of a calculation of a shock or even an acoustic wave moving in the direction of a grid cell diagonal. At the same time, for the acoustic waves propagating in a medium at rest, K. V. Brushlinskii, based on Gelfand's suggestion, constructed the solution of the problem using an interaction of all cells adjoint to one node with the help of the Sobolev's method of functionally invariant solutions. This solution was used in a numerical scheme completely analogous to the 1-D one. After that, the calculations of waves moving in a grid diagonal direction were performed with the help of Brushlinskii's scheme and compared with our scheme. To our surprise and satisfaction, we did not discover any essential differences. After that, only the rough model was employed. We made a lot of efforts to derive a stability criterion needed to choose an admissible time step for a prescribed spatial step. First, using the Fourier method, G.B. Alalykin, K.A. Bagrinovskii and I, arrived at a cubic characteristic equation and derived from it only the necessary condition of stability. Then, together with K.A. Bagrinovskii, we succeeded in obtaining a sufficient condition of stability considering results of 2-D calculation as some averaging of 1-D calculations, or as one says by using a *splitting* approach. This work [24] was published in 1957 where a few not very simple tests were performed with the help of our 2-D code.

The idea to use the *splitting* approach appeared under the influence of investigations of 2-D implicit schemes for the heat equation. These schemes were analogous to ones that were proposed later by J. Douglas and their co-authors. But at that time we refused to use *splitting* for the 2-D heat equation.

Similarly to the construction of the numerical schemes for the gas dynamics and acoustics using non-smooth – discontinuous – solutions, I decided to test proposed splitting schemes for the equation $u_t = u_{xx} + u_{yy}$, taken as a test for the problem of the evolution of a heat impulse released in one grid cell. In other words, I decided to simulate the solution which after some time should not be essentially different from

$$u(x, y, t) = \frac{\text{const}}{t} \exp\left(-\frac{x^2 + y^2}{4t}\right).$$

At least, the level curves of the computed solution should be convex curves – close to circles.

I was very surprised when, during calculations with the Courant number

$$\frac{\Delta t}{(\Delta x^2 + \Delta y^2)} \approx 10,$$

I realized that these level curves turned out to be cross-like at least at the first time steps. This phenomenon forced me to avoid the splitting for the heat equation. However, these investigations led us to use the splitting procedure not only for the stability analysis of gas dynamics numerical schemes but also for the organization of the code structure.

The first 2-D code was constructed in such a way that on the successive steps the fluxes, computed with the help of the 1-D approach, were used at first in one direction and then in the other grid direction. There were no troubles, but later we refused to use splitting in these problems with explicit schemes as V. V. Lucikovich suggested. He said that this refusal allowed to simplify the code and made it more fast-acting. Before we were sure that using the splitting approach led to simplification.

As I mentioned above we had to use the Lagrangian coordinates and turned to the Eulerian coordinates. But at the same time in order to connect the grid with moving boundaries,

we had to make the moving grids as well. In particular, it allowed to include the shock fronts into a special type of boundary. The usefulness of this fact was demonstrated at the calculation of the flow around a sphere [6].

One should remark that in the first variants of our 2-D approaches we constructed meshes and wrote finite-difference formulas on the basis of conservation laws with a lot of caution and carefulness. For example, for cell boundaries, the arcs of logarithmic spirals were used, and the integrals over the cells limited by these spirals were calculated by explicit formulas. Only some years later we began using more simple variants. The hard work to derive the analytic formulas for integrals was performed by K. A. Bagrinovskii and A. V. Zabrodin.

Even in 1-D calculations that were performed in the Lagrangian coordinates we tried to increase the accuracy by looking at the advancement of the strongest shock waves. In order to avoid the spreading of these waves, their coordinates were marked and the grid cells where they were located were divided into two parts. To compute the displacement of a particular wave, the Hugoniot relations were used. After that, we started using the moving grids in the Eulerian coordinates, and the necessity to distinguish the boundary type – shock waves and the boundaries of material layers (contact discontinuity)– disappeared. It simplified the logical structure of the algorithm and allowed us to introduce one more boundary type on Zabrodin's suggestion. These boundaries had an assigned position or moved following a specified law and did not influence the medium flowing across them. They were called Eulerian boundaries.

The grids in regions, limited by boundaries of different types, were attached to these boundaries and computed with the help of simple interpolation formulas. Of course, at each time step, the displacement of boundaries implied the displacement of grid points. The use of codes with such a multi-region structure allowed to increase the accuracy. It was possible not due to the fact that numerical formulas were improved, but because the grid adapted to the solution's structure and strong discontinuities were not smeared. Working with this code I wanted to change the grid calculation based on the interpolating formulas in a geometric region with assigned boundaries into the solution of some differential equations. These equations described a mapping transforming this region into some standard one (for example, into rectangular). G. P. Prokopov and I have studied this problem for seven years (1961-1968) to achieve the first acceptable results [5,25,26].

I am still interested in the classes of mappings for the grid generation although I stopped studying numerical schemes many years ago [27].

From the beginning, G. P. Prokopov and I postulated that the mapping should be defined as a solution of elliptic equation systems. Our main efforts were directed to solve them efficiently. We decided to use a variational approach that was realized with the help of a finite element method. However, we did not perform the first test on calculation of grids in hydrodynamical problems with moving boundaries. Because in this case the elliptic system should be solved on each time step (we were afraid of expensive time-cost). First, we decided to use a variational approach in some stationary problems and applied our ideas to calculate the critical parameters of a nuclear reactor (see [8]). I mentioned above that during these secondary investigations I was interested in computational methods of linear algebra. I was attracted by this problem, and I devoted to it my whole attention.

Only after that we succeeded in finding the solution of stationary problems, we decided to generate grids on each step by solving elliptic equations. The first sufficiently universal code started to work at the end of 1968 – at the beginning of 1969. The first problem computed by it was based on the article [28]. This article contained the talk presented at the International conference on explosion physics (Novosibirsk, 1969) and was devoted to the wave formation at the explosion welding and the analysis of experiments that were carried out at the Novosibirsk Institute of Hydrodynamics.

In September 1969, I moved to Novosibirsk and later did not devote myself to numerical schemes.

I should remark that during the development of the moving grids for 2-D calculations, we tried to use them in 1-D hydrodynamical problems to obtain more exact results. The whole domain was divided into some sub-domains whose boundaries were contact and shock discontinuities, and characteristics. Inside each sub-domain a scheme of the second order was used. It was important for the calculation of rarefaction waves to use many nodes immediately after they emerged (for instance, 50). It provided very high accuracy, and it was possible because of application of implicit numerical schemes.

We carried out the described method together with I. L. Kireeva and L. A. Pliner, and the algorithm and code were written by G. B. Alalikin. Based on this code some principal calculations were made. The method was published in 1970 (see book [1], in russian). I think the book passed unnoticed but I believe the specialists in the area of numerical hydrodynamics can find something interesting even today.

One should mention that at the same time I worked with the characteristics method to adapt it to computer calculations. The result of this activity was the method of characteristics by layers in which not the intersection points of characteristics are calculated, but the coordinates of these characteristics at fixed layers $t = \text{const}$. But after having finished both the method and the code, during the first calculations the method showed its inadequateness. It did not calculate strong rarefaction waves correctly. We did not expect such a situation because the characteristics method supposed to be good in calculation of such waves. Brief communication about this failure was published in [3] and it led me to construct a scheme of the second order to calculate solutions with distinguished discontinuities to which the above cited book is devoted [1].

The scheme for the gas dynamics calculations based on the solution of the Riemann problem began wide-spreading only in 1969, where even three independent presentations were reported during the conference in Novosibirsk. I have already mentioned our presentation. Besides, there was the presentation of M. Ya. Ivanov and A. N. Kraiko from Moscow Central Institute of Aircraft Engines and the presentation of T. D. Taylor and V. S. Mason (USA) about using our scheme to calculate gas-dynamical flow around "Apollo" (see [29,30]). Later, together with our colleagues from Institute of Aircraft Engines we prepared a detailed description of the numerical method and published the book translated in French [31].

4 Conservation laws and thermodynamics

I will touch one more issue appeared during the work on the construction of numerical schemes and related to the concept of generalized solutions of conservative quasilinear equations.

As it was mentioned above the conservation laws of mass, momentum and energy are valid for the numerical solutions computed with the help of my scheme. However the classical solutions (without discontinuities) of gas dynamics equations obey one more additional conservation law – the entropy conservation law. The entropy increases in the case where gas passes through the shock front (discontinuity in the solution). This statement is the Zemplen's theorem, which represents (from the point of view of the theory of quasilinear equations) the postulate included into the definition of generalized solutions. With the help of this postulate the discontinuous solutions satisfying the conservation laws of mass, momentum and energy, so that the entropy of a given material volume is decreasing, are excluded from the number of the generalized solutions. In my scheme, the law of non-decreasing of the entropy is automatically fulfilled because the solutions of the Riemann problem included in this scheme satisfy this law, and also the entropy is increasing in the process of averaging in computational cells. Such averages are performed at the end of each time step in my scheme.

Obviously, I was interested in the description of such quasi-linear equations for n unknowns whose classical solutions satisfy automatically to a $n + 1$ -th conservation law.

Trying to understand which is the answer on this question, I noticed that all nonlinear relations which are present in the hydrodynamical equations are defined by only one nonlinear function – the thermodynamic potential $E(V, S)$. In the Gelfand's lectures on the theory of quasi-linear equations that he gave at the Moscow University [32], the role of in the equalities $E_S > 0$ and $E_{VV} E_{SS} - E_{VS}^2 > 0$ was mentioned. These inequalities in the thermodynamics are used for the gases and liquids if the parameters V, S are far from the phase-transition values. As a problem, I. M. Gelfand suggested to prove that these inequalities provide the well posedness of spreading of sound-waves by acoustic equations for a heat conducting gas. Impressed by this problem I supposed that similar considerations about well posedness or stability (for systems with finite numbers of degrees of freedom) can be put in the base of a well-known thermodynamic theorem on the existence of the integrating multiplier $1/T$ for $dE + p dV$. This theorem is the basis of the entropy definition with the help of the equality $dS = (1/T) (dE + p dV)$. After several months of hard work I succeeded to prove this hypothesis [33]. I found out that the stability, that proves the impossibility to construct the perpetual motion machine of the second kind, is always the consequence of existence of some integral which is dissipated due to the heat transfer. If we study only the stability of small oscillations (i.e. describing the evolution of a system by linear equations), the dissipating integral appears to be a quadratic form with a symmetric and positive definite coefficient matrix. The symmetry of this matrix leads to the equalities from which the existence of a universal integrating multiplier is derived. In my article [33] (see also § 22 in the book [23]) the drafts of the perpetual motion machine of the second kind are presented in the case where the universal integrating multiplier does not exist.

After finishing the work [33], in order to understand the reasons for which the three equations have the "extra" fourth conservation law, it was natural to represent the hydrodynamical equations in the Lagrangian coordinates (they are used for classical solutions)

$$\begin{aligned}\frac{\partial V}{\partial t} + \frac{\partial u}{\partial x} &= 0, \\ \frac{\partial u}{\partial t} + \frac{\partial E_V(V, S)}{\partial x} &= 0, \\ \frac{\partial S}{\partial t} &= 0,\end{aligned}$$

and derive the fourth conservation law as their linear combination

$$\begin{aligned}0 &= \frac{\partial(E(V, S) + u^2/2)}{\partial t} + \frac{\partial(u E_V(V, S))}{\partial x} \\ &\equiv E_V(V, S) \left[\frac{\partial V}{\partial t} + \frac{\partial u}{\partial x} \right] + u \left[\frac{\partial u}{\partial t} + \frac{\partial E_V(V, S)}{\partial x} \right] + E_S \frac{\partial S}{\partial t}.\end{aligned}$$

Obviously, such an equality representing a linear dependence between four conservation laws can be solved relatively to any of them. In particular, the entropy conservation law $\frac{\partial S}{\partial t} = 0$ can be presented as a linear combination of the conservation law for the specific volume

$$\frac{\partial V}{\partial t} + \frac{\partial u}{\partial x} = 0,$$

the conservation law of the momentum

$$\frac{\partial u}{\partial t} + \frac{\partial E_V}{\partial x} = 0,$$

and the conservation law of the energy in the following way

$$0 = \frac{\partial S}{\partial t} = -\frac{E_V}{E_S} \left[\frac{\partial V}{\partial t} + \frac{\partial u}{\partial x} \right] - \frac{u}{E_S} \left[\frac{\partial u}{\partial t} + \frac{\partial E_V}{\partial x} \right] + \frac{1}{E_S} \left[\frac{\partial(E + u^2/2)}{\partial t} + \frac{\partial(u E_V)}{\partial x} \right].$$

The last equality is possible due to the relation between the differentials

$$dS = -\frac{E_V}{E_S} dV - \frac{u}{E_S} du + \frac{1}{E_S} d\left(E + \frac{u^2}{2}\right).$$

It is convenient to use the following form

$$d\left[S + \frac{E_V}{E_S} V + \frac{u^2}{2E_S} - \frac{1}{E_S}\left(E + \frac{u^2}{2}\right)\right] = V d\frac{E_V}{E_S} + u d\frac{u}{E_S} - \left(E + \frac{u^2}{2}\right) d\frac{1}{E_S},$$

and to introduce the notation

$$\begin{aligned} L &= S - \frac{1}{E_S}\left(E + \frac{u^2}{2}\right) + \frac{V E_V}{E_S} + \frac{u^2}{2E_S} = \frac{1}{E_S} [S E_S + V E_V - E], \\ q_1 &= \frac{E_V}{E_S}, \quad q_2 = \frac{u}{E_S}, \quad q_3 = -\frac{1}{E_S} = -\frac{1}{T}. \end{aligned}$$

As a result, we have the equalities that relate derivatives L_{q_i} to the quantities appearing in the hydrodynamical equations under the derivative $\frac{\partial}{\partial t}$

$$L_{q_1} = V, \quad L_{q_2} = u, \quad L_{q_3} = -(E + u^2/2),$$

and the relations between the differentials dS , dV , du , $d(E + u^2/2)$ in an elegant form, on which the well-known Legendre's transform in the theory of convex functions is based

$$d(q_1 L_{q_1} + q_2 L_{q_2} + q_3 L_{q_3} - L) = L_{q_1} dq_1 + L_{q_2} dq_2 + L_{q_3} dq_3.$$

It is convenient to introduce one more function of q_1, q_2, q_3

$$M = -\frac{q_1 q_2}{q_3},$$

such that

$$\begin{aligned} M_{q_1} &= -\frac{q_2}{q_3} = u, \\ M_{q_2} &= -\frac{q_1}{q_3} = E_V, \\ M_{q_3} &= -\frac{q_1 q_2}{q_3^2} = u E_V, \\ M - q_1 M_{q_1} - q_2 M_{q_2} - q_3 M_{q_3} &= 0. \end{aligned}$$

In this case the hydrodynamical equations have the following form

$$\frac{\partial L_{q_i}}{\partial t} + \frac{\partial M_{q_i}}{\partial x} = 0, \quad i = 1, 2, 3.$$

They consist of three conservation laws, and the fourth (additional) one

$$\begin{aligned} &\frac{\partial}{\partial t}(q_1 L_{q_1} + q_2 L_{q_2} + q_3 L_{q_3} - L) - \frac{\partial}{\partial x}(q_1 M_{q_1} + q_2 M_{q_2} + q_3 M_{q_3} - M) \\ &\equiv \frac{\partial}{\partial t}(q_1 L_{q_1} + q_2 L_{q_2} + q_3 L_{q_3} - L) = 0, \end{aligned}$$

coincides with the conservation law of entropy $\frac{\partial S}{\partial t} = 0$. Afterward it was not difficult to obtain for other classical equations of mathematical physics, even multidimensional, the standard representation

$$\frac{\partial L_{q_i}}{\partial t} + \frac{\partial L_{q_i}^j}{\partial x_j} = 0.$$

I succeeded in writing in a similar form the gas dynamics equations in the Eulerian coordinates. I was happy with the fact that if the generating "*thermodynamic potential*" $L = L(q_1, q_2, \dots)$ is convex, these equations can be rewritten in the form of the Friedrichs's symmetric hyperbolic system

$$L_{q_i q_k} \frac{\partial q_k}{\partial t} + L_{q_i q_k}^j \frac{\partial q_k}{\partial x_j} = 0,$$

with a positive definite matrix of coefficients at derivatives ∂q_i on t . K. O. Friedrichs showed that for such systems the Cauchy problem is well-posed if some conditions on the smoothness of initial data are true.

So, my hopes to discover the connection between well-posedness and the laws of phenomenological thermodynamics have been realized.

I described all my achievements in the article that was sent to the journal "Uspekhi Matematicheskikh Nauk", but it was not published because a reviewer decided that it did not have a mathematical content.

After that I was dealt a new severe blow. I decided to use the obtained equations by introducing into them small additional dissipation terms. I wanted to confirm that the discontinuous solutions, after introducing any small viscosities, are just "smeared" in a thin stripe, and that the limit solutions (generalized solutions of equations with zero viscosity) do not depend on the form of these viscosities. Considering solutions in the form of travelling waves $q_i = q_i(\xi)$, $\xi = (x - \omega t)/\varepsilon$ for equations

$$\frac{\partial L_{q_i}}{\partial t} + \frac{\partial M_{q_i}}{\partial x} = \frac{\partial}{\partial x} \left[\varepsilon b_{ik}(q) \frac{\partial q_k}{\partial x} \right].$$

I could propose an obvious geometric interpretation for ordinary differential equations for $q_i(\xi)$. This interpretation led to a construction of systems of hyperbolic conservation laws for which admissible discontinuous solutions satisfied the entropy increasing law, and which depend on what kind of small dissipative terms we introduced to smooth them. In physical problems the real dissipative processes can differ from the numerical dissipation that depends on the numerical scheme. Soon, B. F. Diachenko constructed the example in which different numerical approximations led to different numerical solutions [34].

I was very upset that I could not justify all hypotheses lying in the background of the numerical scheme. My work with the description of this example was presented in "Doklady AN SSSR" [35], [36] by I. G. Petrovskii. Before the article was published, I presented it on the seminar where R. Courant and P. D. Lax participated, and visited Moscow for the first time.

Later, in Novosibirsk, together with my colleagues I continued the investigations on conservation laws and their connections with the thermodynamics. The review of a part of these investigations was included into the paper [22] that I presented in 1986 in St.-Etienne at the Conference on hyperbolic equations. I should also mention important studies [37], [38] on this issue performed by P. D. Lax and K. O. Friedrichs. Last years these studies were continued and presented by me and E.I. Romenskii in Lisbon, Lake Tahoe (USA, Nevada), Paris [39-41]. Our work [42] (in collaboration with T. Yu. Mikhailova) was also devoted to this topic. The works [41],[42] showed unexpected connection between formally overdetermined systems of conservation laws in mathematical physics and the theory of representations of the rotation group.

I should notice a recent work [43] in which the estimates of the entropy growth for the systems of conservation laws in the form described above are investigated. The author of this work could connect these estimates with the *variation* of solutions. It seems to me that this original way of definition of such a *variation* is very promising. For this definition it is not important if the problem is one-dimensional or multi-dimensional.

5 Conclusion

In this note I tried to describe the intensive work in the field of numerical hydrodynamics in which I was involved by my supervisors I. G. Petrovskii and I. M. Gelfand, and the result was the development of *Godunov's scheme*.

I should emphasize the influence of the whole scientific community within I worked. Of course, different approaches to the numerical hydrodynamics were elaborated by many other research groups and some of these groups belonged to the Institute where I worked. The scientists who participated in these groups are K. I. Babenko, V. V. Rusanov, I. M. Gelfand, V. F. Diachenko, A. A. Samarskii, N. N. Janenko, B. L. Rozhdestvenskii, and others. My goal was not to describe the whole history of this subject but only present the part in which I participated.

Various discussions with outstanding physics theoreticians of that time such as Ya. B. Zeldovich, A. D. Sakharov, D. A. Frank-Kamenetskii, Yu. B. Hariton, as well as members of the experimental group of L. V. Altshuler were very essential for me. I have already remarked that the comments of physicists were, as a rule, very critical. They stimulated the detailed analysis of all numerical effects and their reasons, and led to modifications of the method. The specific problem for a steady flow around a body was suggested to me by G. I. Petrov.

I wanted to demonstrate how the set of the principal scientific issues emerged during that initial period of the development of the computational fluid dynamics. Many of these issues are still unresolved even today.

6 References

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Appendix

Experimental study of a disparity between order of approximation and accuracy ¹

We present a method allowing an efficient estimation of the order of the weak convergence, which is based on generalized solutions of hyperbolic systems of conservation laws. The idea of the method was suggested by S. K. Godunov and V. S. Ryabenkii. The method is based on the experimental estimation of the convergence rate of the first integrals of numerical solutions which are calculated over domains with singularities of the approximated exact solution. The analysis of the accuracy of the Harten's TVD-scheme with the second order approximation on smooth solutions shows that only the first order of convergence occurs in the problem of dam breaking with creation of a bore and a smooth rarefaction wave. It results in the decreasing of the order of strong convergence in smooth parts of exact solutions behind the wave front. The result obtained is in contradiction with a wide-spread opinion according to which the monotonic numerical schemes of higher order of approximation on the smooth solutions conserve a higher order of local convergence on smooth solutions of quasi-linear hyperbolic conservation laws.

Let us consider the Cauchy problem for hyperbolic system of quasi-linear conservation laws

$$u_t + f(u)_x = 0, \quad u(0, x) = u_0(x), \quad x \in \mathbb{R}, \quad (1)$$

where $u_0(x)$ is a m -dimensional piecewise continuous vector-function and $f(u)$ a smooth flux function. We suppose that the problem (1) has a unique stable generalized solution $u(t, x)$. The numerical solution is calculated with an explicit two-layer in time and symmetric in space conservative scheme

$$v_j^{n+1} = v_j^n - \lambda_n (\bar{f}_{j+1/2}^n - \bar{f}_{j-1/2}^n), \quad v_j^0 = u_0(jh), \quad j \in \mathbb{Z}, \quad (2)$$

where $\bar{f}_{j+1/2}^n = \bar{f}(v_{j-k+1}^n, \dots, v_{j+k}^n)$, $\bar{f}(u, \dots, u) = f(u)$, for all $u \in \mathbb{R}^m$, $v_j^n = v(t_n, jh)$, $t_0 = 0$, $t_n = \tau_0 + \tau_1 + \dots + \tau_{n-1}$, $\lambda_n = \tau_n/h$, τ_n is the time step at n -th time layer t_n , h is the constant spatial step, \bar{f} is the continuous function of numerical flux. The time step τ_n is calculated from the Courant condition $\tau_n \leq \tau_n^{\max} = zh / \max_{i,j} |a^i(v_j^n)|$, where $z = 0.5$ is a safety factor, $a^i(u)$, $i = 1, \dots, m$ are the eigenvalues of Jacobi matrix f_u in (1). Let us fix a number a , $a \in \mathbb{R}$ and introduce the integrals

$$U^a(T, x) = \int_a^x u(T, y) dy, \quad V_h^a(T, x) = \int_a^x v_h(T, y) dy. \quad (3)$$

The numerical solution $v_h(T, x)$ converges weakly to the exact solution $u(T, x)$ with r -order within segment $[a, x] \subset \mathbb{R}$ if

$$V_h^a(T, x) - U^a(T, x) = C h^r + o(h^r), \quad (4)$$

where C does not depend on h .

If $[a, x]$ does not contain singularities of the exact solution, the order of weak convergence coincides with the order of a local convergence on smooth solutions, i.e. equals to 2 in our case. Otherwise, the order of weak convergence is less than 2, because the TVD schemes do not have second order of weak approximation on discontinuous functions.

Let us estimate the order of weak convergence r in the case where an exact discontinuous solution of the problem (1) is unknown in advance. To calculate the order of weak convergence (based on the Runge's rule) it is enough to have three numerical results with

¹In this Appendix the results obtained by V.V. Ostapenko (Lavrentev Institute of Hydrodynamics SO RAS, Novosibirsk) are used.

rather small spatial steps $h_1 = h, h_2 = h/2, h_3 = h/4$. For each step the property (4) is satisfied, hence

$$\delta V_i = |V_{h_i}^a - V_{h_{i+1}}^a| = |C| (h_i^r - h_{i+1}^r) + o(h^r), \quad i = 1, 2. \quad (5)$$

Therefore, we obtain with the accuracy $o(h^r)$

$$\frac{\delta V_1}{\delta V_2} = \frac{h_1^r - h_2^r}{h_2^r - h_3^r} = \frac{1 - (1/2)^r}{(1/2)^r - (1/4)^r} = 2^r,$$

from which it follows that

$$r = \log_2 \frac{\delta V_1}{\delta V_2}. \quad (6)$$

Below we present the results of a numerical calculation of errors (5) and the order of accuracy (6) based on the TVD-scheme in the problem of dam breaking in a channel of non-constant depth.

As a test scheme one chooses one of the TVD-schemes suggested by Harten ². This scheme is applied to the numerical solution of the Saint-Venant equations (shallow water equations). They are equivalent to the equations of the polytropic gas with polytropic exponent $\gamma = 2$ and have the following form

$$u_t + f(u)_x = 0, \quad u = \begin{pmatrix} H \\ q \end{pmatrix}, \quad f(u) = \begin{pmatrix} q \\ q^2/H + g H^2/2 \end{pmatrix},$$

where H and q are the depth and the flux, respectively, g is the gravity (in calculations $g = 10$).

In the Figures 1-4 for $T = 0.2$ one can observe the results of the calculation of the Cauchy problem with discontinuous initial data

$$H(0, x) = \begin{cases} 10, & x \leq 3.5, \\ 2 - th(x - 5), & x > 3.5, \end{cases} \quad (7)$$

$$q(0, x) = 0, \quad x \in \mathbb{R}. \quad (8)$$

In these calculations, $h_1 = h = 0.1, h_2 = h/2 = 0.05, h_3 = h/4 = 0.025$.

The results of the calculations are presented in Figure 1: circles correspond to the basic grid with step h_1 , the solid line to the grid with step h_3 ; the dotted line corresponds to the initial position of the water level given by function (7).

Figures 2–3 are the error, as defined by (5), and the order of accuracy given by relation (6); $a = 12$ in relation (3). From these plots, one can see that, when $x > 6$, i.e. when the segment of integration $[a, x]$ lies entirely in the smooth part of the solution just before the shock wave front, the order of weak convergence $r(x)$ equals 2. When $x < 5$ and when $[a, x]$ contains the front of a discontinuous wave, then $r(x) \approx 1$, and the TVD-scheme (2) has approximately only the first order of accuracy for the Cauchy problem (7)–(8).

In Figure 4, the function

$$r_0(x) = \begin{cases} R(x), & R(x) \leq 3, \\ 3, & R(x) > 3, \end{cases}$$

is plotted where

$$R(x) = \log \frac{\delta v_1(x)}{\delta v_2(x)}, \quad \delta v_i(x) = |v_{h_i}(T, x) - v_{h_{i+1}}(T, x)|, \quad i = 1, 2,$$

that presents the order of the local strong convergence of the numerical solution. As one can see from Figure 4, the calculation domain is divided into three isolated parts by singularities

²J.Comp.Phys.1983, V.49, P.357-393.

of the exact solution (inside every part the order of local convergence is changed in a random way). Inside each part there is a different order of the local convergence. The order of the local convergence of the TVD-scheme on different smooth parts is quite different, and, generally speaking, less than the order of approximation on the smooth solutions (see Fig.4).

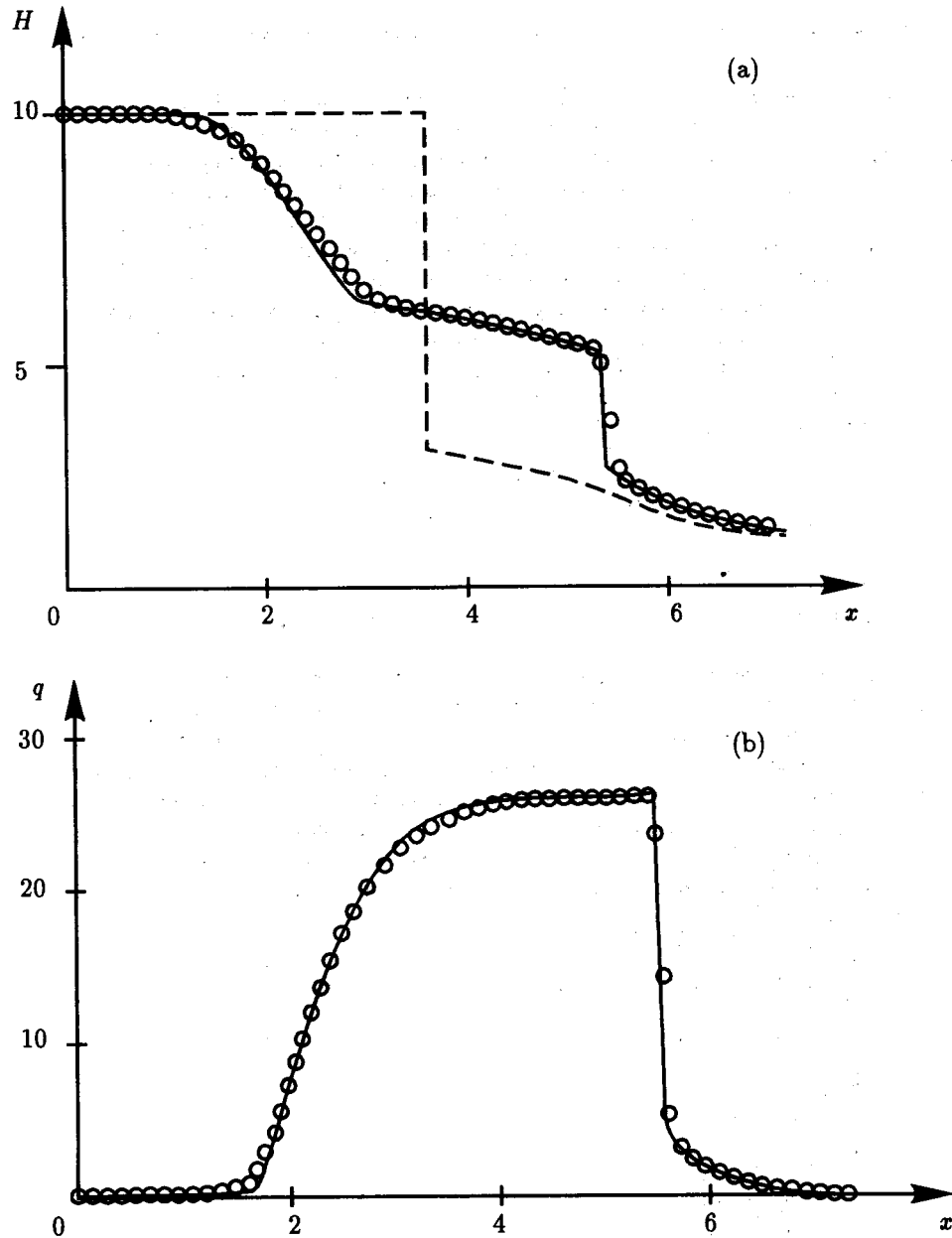


Figure 1: Comparison of an exact and a numerical solution

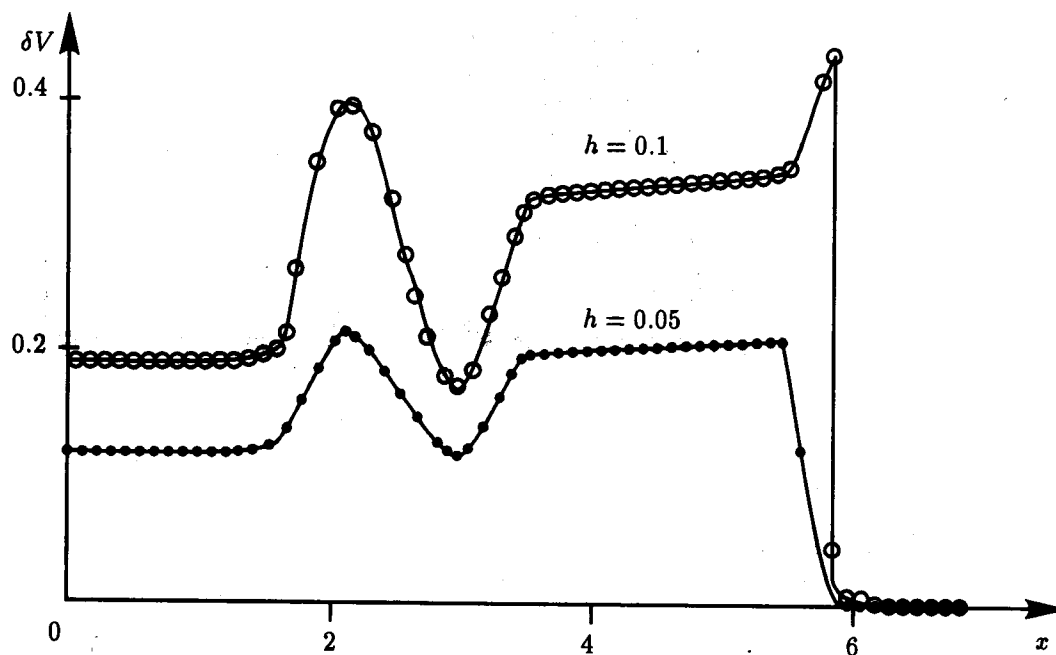


Figure 2: Disbalances of the integrals of a numerical solution

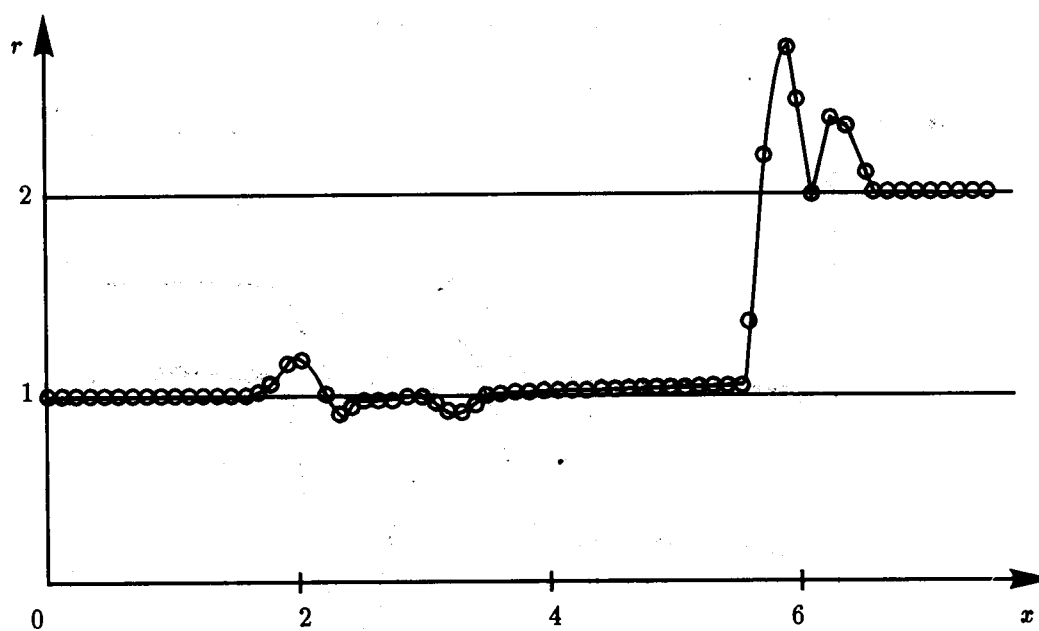


Figure 3: The weak convergence order r

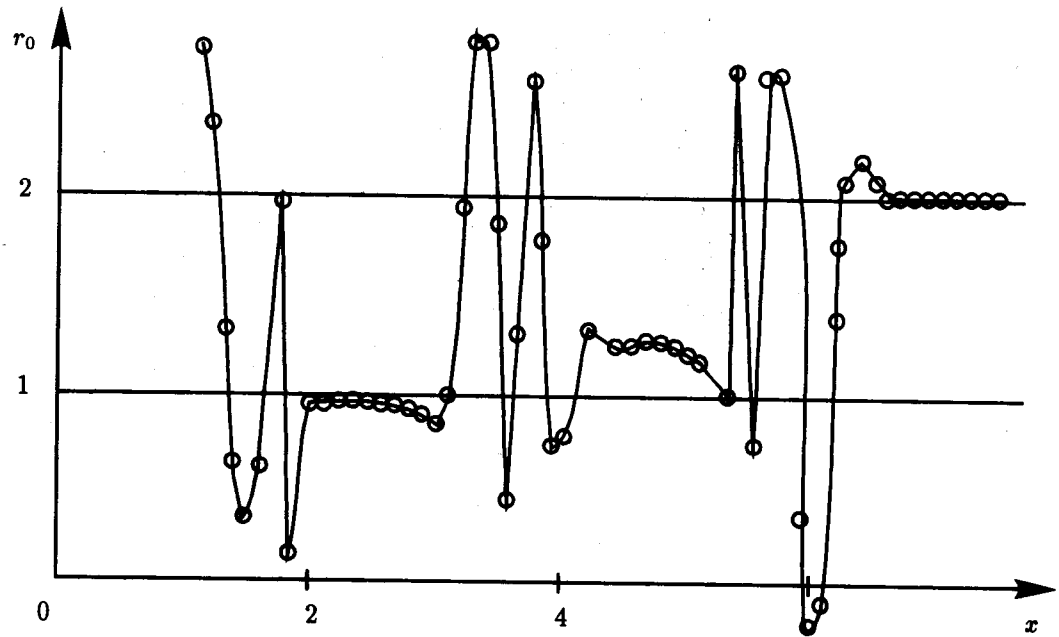


Figure 4: The strong convergence order $r_0(x)$



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