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SPECIAL ARTICLE

Reminiscences about Difference Schemes[1]

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FOREWORD

In these notes, I will tell how in 1953–1954 the first version of the "Godunov's scheme" was invented and how it was modified in the subsequent works by myself (until 1969) and by others at the Institute of Applied Mathematics in Moscow (now named after its founder, academician M. V. Keldish).

Parallel to the modifications which I will describe below (Sections 1, 2), other algorithms were being developed as well at that time, in particular second-order accurate methods for gas-dynamical flows with a small number of strong and weak discontinuities [1, 27, 26]. Our research activity was related to performing a large number of calculations. The first codes for this purpose were written by V. V. Lucikovich. As the problems became more complex, more artful techniques were required for splitting the computational domain into sub-domains. A. V. Zabrodin was a master in this field. Usage of such splitting techniques lead to the necessity to make the grid generation automatic.

Between 1961 and 1968, together with G. P. Prokopov, we worked long and hard on the methodology for the generation of moving grids, which in 1968–1969 were included into the commercial codes by A. V. Zabrodin and programmers G. M. Novozhilova and G. B. Alalikin [39, 13, 31]. The problems that arose in the grid generation focused our attention on the solution of elliptic systems [20, 38]. Later these methods were used in elliptic spectral problems [30, 21], which attracted my attention to the problems of numerical linear algebra. A whole host of surprising observations made at that time provided a source of seminar discussions at Moscow University and, after 1969, at Novosibirsk University for years to come. These discussions resulted in the development of spectral dichotomy methods [18, 16]

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and high-precision methods for the calculation of singular eigenvectors, which became the basis for our books [18, 32]. It would be hard to guess that this research originated from the development of the methods for gas-dynamical calculations and the grid generation for these calculations.

I started to study the theory of differential equations at Moscow University at the seminars of I. M. Gelfand and I. G. Petrovskii. The latter drew my attention to the problems of gas dynamics and suggested the use of relaxation methods for the study of flows with both subsonic and supersonic regions. My master's thesis was devoted to this issue; I considered the relaxation of a flow in a nozzle (but only in the subsonic case and with the use of some artificial time derivatives introduced into Chaplygin's equation). A version of Petrovskii's idea about relaxation to a steady state, applicable for practical problems, was published in 1961 [31]. This publication was based on a much later calculation performed with our algorithm. The technical formulation of this algorithm was the essence of the master's thesis of G. P. Prokopov, which I supervised. The code itself was written by G. N. Novozhilova.

The development of difference schemes for gas dynamics was parallel to the attempts to formulate and adapt the concept of a generalized solution for quasi-linear systems of equations. Usually the hypothesis about possible definitions and properties of generalized solutions preceded the construction of the difference schemes which tried to make use of those properties. At the same time, I was trying to justify the hypothesis. To my greatest frustration those attempts were unsuccessful, and even worse, they often resulted in contradictory examples. Not surprisingly, those examples put me in despair. Meanwhile, the difference scheme, or more precisely its modification utilizing Euler's coordinates and moving grids following the course of principle strong and weak discontinuities, was actively used in commercial calculations.

1. HOW THE SCHEME WAS INVENTED

In the autumn of 1953, M. V. Keldish and I. M. Gelfand asked me to develop a version of a method published by J. Von Neumann and R. D. Richtmyer (1950). Their method is based on the introduction of artificial viscosity into the gas-dynamics equations. I had been strongly encouraged to finish the development of a suitable algorithm for commercial purposes by the spring of 1954, the time when the first electronic computer, "Strela" (Arrow), was to arrive at our institute. It was to be the very first one of its kind in mass production.

I was informed that a possible version of the required algorithm was already prepared in our institute by A. I. Zhukov. Being allowed to read his report, I was given the freedom to modify his methods or suggest something new. From the point of view of the institute's senior scientists, it was critical to advance the research frontier in computational gas dynamics so as to meet the deadline.

The method suggested by Zhukov was exactly the same as the Lax scheme, published a year later [37]. However, Zhukov's report had a number of conjectures, formulated as truth-like hypotheses, upon which the construction of the scheme was based. Looking back, I can now say that some of them turned out to be wrong. However, when first reading the report, I did not doubt these hypotheses. I, therefore, decided to use them in my work.

The principal difference between the method proposed by Zhukov and that of Von Neumann and Richtmyer is that Zhukov did not use artificial viscosity. As a result of his numerical experiments, Zhukov concluded that the viscous smearing of the shock waves

occurs automatically in the finite-difference solution due to the discrepancy between the discrete approximation and the exact continuous differential equations. He suggested using *numerical viscosity* to represent the deviations of the difference scheme from the continuous equations, resulting in the formulation of the *first differential approximation.*[2]

Zhukov tried to use second-order schemes first, but they produced strong oscillations near the shock front. He explained them with the help of the exact solutions (in terms of Airy functions) of the linearized equations with artificial viscosity approximating the numerical viscosity of the difference scheme. Thus, Zhukov came to the conclusion that it is impossible to use second-order accurate schemes and concentrated on the development of a first-order scheme, using both the simplest quasi-linear Burgers' equation and gas dynamic equations in Lagrangean coordinates as the models. All his attention was concentrated on studying the solutions of a problem with a steadily moving shock front. Using the first differential approximation, this problem can be reduced to a set of ordinary differential equations whose solutions can be compared with the results of the finite difference calculations. Using these comparisons, Zhukov formulated a necessary condition which should be satisfied by any difference scheme. The condition was that the equations of the first differential approximation should have the form of conservation laws. However, the condition was given in the form of a hypothesis as both a necessary and sufficient condition.

I did not question this statement and used it as a cornerstone in my attempts to build a second-order scheme which did not exhibit oscillations. I started examining different second-order schemes for which the exact conservation laws were not satisfied, but those of the first differential approximation were. All schemes were checked via the calculation of a single solution chosen as a typical model problem.

Eventually, I found a rather satisfactory scheme. It took about three months of intensive work. N. M. Zueva had been helping me with analytical manipulations and evaluation of the residual terms, while the numerical calculations were performed by V. V. Paleichik and two of her students who were learning the art of using mechanical adding machines made by Mercedes. Keldish and Gelfand payed strong attention to this research and listened to the progress reports biweekly.

In the next phase of research, the robustness of the scheme was to be tested in calculations with different spatial step sizes and for a variety of different solutions. However, studying the dependence of the solution on the spatial step size, we discovered that our previous three months of work were completely misdirected.

In order to explain the obstacles we faced, I have to tell about another hypothesis from Zhukov's report. He compared the results of integration of the first differential approximation with the results of finite-difference calculations and noticed a discrepancy. He suggested that this discrepancy would go away as the spatial step approaches zero.

I decided to verify this statement and asked V. V. Paleichik to perform the corresponding calculations. One of her students was doing the calculations with one possible step size, while another with one-half of that step. In just five to ten minutes Paleichik started to reproach me with indignation for this useless experiment. After the first stage, the results of both calculations turned out to be identical, and it could not be otherwise since the spatial step did not appear in the formulas by itself. The scheme depended only on the ratio of time to spatial step, which we did not change in order to keep Courant's number constant. Since the finite-difference profiles do not depend on the spatial step size, it is impossible that they

[2] In western literature, this is referred to as the lowest-order *modified equation.*

would approach the solutions of the first differential approximation as the step goes to zero. Comparing the exact and finite-difference shock speeds a difference of 3 to 4% was noted, leaving no hope that this difference would decrease for smaller spatial steps.

As is natural, the above observations brought me to a stressed condition and made me reconsider all the previous points of view.

First of all, it became obvious that a difference scheme should provide a correct speed for a steadily moving shock and correct values of the state variables on either side of the shock, *even for a step size equal to 1*. The hope that the precision in shock wave calculations could be gained through smaller spatial steps disappeared completely.

Thus, instead of using simplifications resulting from the first differential approximation and its conservation laws, solving the problems required that the *exact conservation laws* be satisfied. Following this idea, it was suggested to write the approximation to the equations

$$\frac{\partial u}{\partial t} + \frac{\partial p(v)}{\partial x} = 0,$$

$$\frac{\partial v}{\partial t} - \frac{\partial u}{\partial x} = 0$$

so that the difference equations would also have the form of conservation laws,

$$\frac{u_n^{m+1} - u_n^m}{\Delta t} + \frac{P_{n+1/2}^m - P_{n-1/2}^m}{\Delta x} = 0,$$

$$\frac{v_n^{m+1} - v_n^m}{\Delta t} - \frac{U_{n+1/2}^m - U_{n-1/2}^m}{\Delta x} = 0.$$

The gas speed is described by both u_n^m and $U_{n+1/2}^m$. Similarly, the specific volume v and its related quantity, pressure $p(v)$, are approximated by both v_n^m and $P_{n+1/2}^m$, respectively. The formulas relating the lower and upper case letters determine the scheme we are considering. The scheme of choice should always provide a smooth profile of the discrete shock wave. From this monotonicity property together with the difference conservations laws it can be deduced that the shock is moving with a correct speed and the values on the left and right of the shock are related by the well-known Hugoniot relations.

In the first stage I decided to achieve smooth profiles for weak waves, i.e., for the equations of acoustics, which can be considered as gas dynamics with the simplest equation of state $p(v) = -a^2 v$ ($a^2 = \text{const}$). In this case the shocks become jumps in the Riemann invariants $u \pm av$, and the equations are reduced to a canonical form

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

I decided to choose difference schemes which could be reduced, at least for this simplest case, to independent equations for the Riemann invariants $u \pm av$. I started with a known and widely used simple scheme preserving monotonicity of the Riemann invariants. This monotonicity was a guarantee for the smoothness of shocks, which was what I needed. In any case, I was unable to come out with something else and time was running out—they had already started to put together "Strela," delivered from the plant. In addition, I was able

to show that in the linear case only first-order schemes can preserve monotonicity. So I stopped trying to devise a second-order method.

The chosen scheme in the simplest case can be written as

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

which becomes a scheme in discrete conservation form if we define

$$P_{n+1/2}^m=-a^2\frac{v_{n+1}^m+v_n^m}{2}+a\frac{u_{n+1}^m-u_n^m}{2}=\frac{p\left(v_{n+1}^m\right)+p\left(v_n^m\right)}{2}+a\frac{u_{n+1}^m-u_n^m}{2},$$
$$U_{n+1/2}^m=\frac{u_{n+1}^m+u_n^m}{2}+a\frac{v_{n+1}^m-v_n^m}{2}=\frac{u_{n+1}^m+u_{n-1}^m}{2}-\frac{p\left(v_{n+1}^m\right)-p\left(v_n^m\right)}{2a}.$$

It was decided to use this scheme in the general nonlinear case. However, it was then necessary to replace the constant a in the formulas for $P_{n+1/2}^m$ and $U_{n+1/2}^m$ with some function of the solution $a_{n+1/2}^m$. The most natural guesses were

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

We investigated these formulas in experimental calculations, in which we checked the monotonicity of a shock wave for different values on its left and right. Those values were always related by the Hugoniot conditions.

Proceeding with these calculations and observing the shock profiles, I started experimenting with other formulas for $a_{n+1/2}^m$. In particular, requiring that monotonicity is preserved even at the first step I was able to find a reasonable interpolation formula for $a_{n+1/2}^m$ which led to the most acceptable results.

Here I have to add a few details to my story to remove some of the simplifications I have made. As a matter of fact, the experiments I am describing were mostly performed not on the simplest model for gas-dynamics described above, but on the following system of three equations

$$\frac{\partial u}{\partial t}+\frac{\partial p(v,E)}{\partial x}=0,$$
$$\frac{\partial v}{\partial t}-\frac{\partial u}{\partial x}=0,$$
$$\frac{\partial(E+u^2/2)}{\partial t}+\frac{\partial(pu)}{\partial x}=0,$$

for which the difference conservation laws were written as

$$\frac{u_n^{m+1}-u_n^m}{\Delta t}+\frac{P_{n+1/2}^m-P_{n-1/2}^m}{\Delta x}=0,$$

$$\frac{v_n^{m+1}-v_n^m}{\Delta t}-\frac{U_{n+1/2}^m-U_{n-1/2}^m}{\Delta x}=0,$$

$$\frac{(E+u^2/2)_n^{m+1}-(E+u^2/2)_n^m}{\Delta t}+\frac{P_{n+1/2}^m U_{n+1/2}^m-P_{n-1/2}^m U_{n-1/2}^m}{\Delta x}=0.$$

The search for an interpolation formula for $a_{n+1/2}^m$, in this case, is equivalent to the search for expression for $P_{n+1/2}^m, U_{n+1/2}^m$ via $u_n^m, v_n^m, E_n^m, u_{n+1}^m, v_{n+1}^m, E_{n+1}^m$. We were able to find an acceptable variant rather quickly—in two or three weeks. It is important to notice that in those formulas the role of $a_{n+1/2}^m$ was played by an expression

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

which depends on $P_{n+1/2}$. (In these experiments the equation of the state was $E=\frac{pv}{\gamma-1}$.) It occurred to me that I had seen this expression somewhere in the literature and I tried to recall where.

Not long before that time, a book by L. D. Landau and E. M. Lifshitz "The Mechanics of Continuous Media" had been published. It was in the chapter about the break up of an arbitrary discontinuity (the Riemann problem) that I had seen the above expression. I realized I just had to introduce some minor corrections into my interpolation formulas, important only for strong rarefaction waves, to give the final form to my scheme. This work was finished in the March of 1954. In the end of March, V. V. Lucikovich was added to our group. He was to write the program on the basis of the technical requirements which he and I had written using helpful recommendations from K. A. Semendjaev. In the end of April I took two weeks of vacation and on the 5th of May we started experimental and applied calculations.

On the 4th of November 1954 I defended my Ph.D. thesis, which was the description of my scheme. However, it was only in 1959 when it was published in the literature. Until that time I had been trying to submit it to several journals, but without any success. For example, *Applied Mathematics and Mechanics* rejected the article as purely mathematical and having nothing to do with mechanics. One mathematical journal (I do not remember which one exactly) rejected it for the exact opposite reason. After that Petrovskii helped me to publish the work in *Mathematicheskii Sbornik* where he was a member of the editorial board [8].

I read the paper by P. D. Lax [37] only after my thesis defense. His scheme is identical to that of Zhukov, but his paper did not have any suspicious conjectures, which were numerous in Zhukov's report. It was the critical analysis of those conjectures which resulted in my scheme. If I would have read Lax's paper a year earlier, "Godunov's Scheme" would never have been created.

2. PROBLEMS OF APPROXIMATION AND EFFECTIVE ACCURACY

Of course, the work on the scheme invented in 1954 was going on at a later time as well. The final users of our calculations were always very suspicious about it.

In our institute, actually to be precise, in Stekhlov's Institute, from which Keldish's Institute separated in 1953, basic procedures for hydrodynamic calculations were established by K. A. Semendjaev long before I came there. They were performed by a large group of exclusively female operators on Mercedes-brand electrical adding machines using the method of characteristics. Particular attention was paid to the form of the tables where the results were recorded and to the minimization of intermediate records there. This optimization was achieved by an efficient use of the special memory clusters of the adding machines. Final results were always carefully plotted and checked.

The technique of these calculations was very well developed. The operators played on the keys of the calculators like pianists while actively discussing household matters and other problems that usually excite female interest. They were also teasing all the new and shy young researchers of the theoretical subdivision, a group to which I, myself, belonged. We were disparagingly referred to as "that science." They often acidly remarked that our pseudo-scientific explanations for the various numerical troubles which frequently hindered the calculation usually turned out to be useless. One should keep in mind that they were paid for the volume of calculations, as determined by the number of filled-up lines in the tables. Any calculations with errors were not taken into account.

The visual representation of the results on graph paper always was of excellent quality. It displayed easy-to-read images of velocity, pressure, and density fields as well as the trajectories of the contact discontinuities. Carefully plotted characteristics allowed one to see the domains of influence for the interesting parts of the initial conditions.

Our customers—physicists and engineers—were used to the perfect form of the calculations' output so they were unhappy with the first results of computer calculations on the basis of difference schemes. As it is well known now, finite-difference calculations of discontinuous solutions of gas-dynamic equations have plenty of purely numerical "micro-structure," which looks like errors, distorting the flow field. The comparisons of computer output with the "smoothed out" results of hand-made calculations made a negative impression on our customers and led to the claims that the code had serious errors or the calculations were made with the wrong initial data. We had to invest much effort into the analysis of these complaints. Some of them found satisfactory explanations; in other cases, we had to specify some post-processing routines to remove most of these "parasitical" effects or, occasionally, to modify our schemes somehow.

Now I will give two examples of this kind that I find particularly interesting.

The calculations of strong isentropic rarefaction waves with my scheme resulted in a noticeable increase in the entropy; this problem caused a lot of dissatisfaction with the results of our calculations. A considerable decrease of spurious entropy production was discovered three to four years later (in 1957–1958), when we started to perform two-dimensional calculations. Those problems are usually hard to formulate in Lagrangean coordinates, so we had to switch to the Eulerian description. This actually required additional sophistication—we had to start using moving grids. However, the main idea of the method—to use the exact solutions of the Riemann problem—was still applicable, although in a less straightforward way. The first test cases for the just-written two-dimensional programs were one-dimensional calculations which could be compared with our old results. To our great surprise the new two-dimensional codes based on Euler coordinates produced much less "parasitical" entropy in the rarefaction waves.

The explanation for this phenomenon is that Lagrangean coordinates are not very well suited (even in the one dimensional case) for the formulation of "generalized solutions" of

gas-dynamical equations. For a certain type of initial conditions, these equations allow the formation of vacuum zones, which appear in Lagrangean coordinates as delta functions. Singularities of this type are usually not expected in the solutions and are very badly modeled numerically. The analysis showed that even a significant reduction of the step size in Lagrangean coordinate around a strong rarefaction does not necessary imply that the distance between the two adjacent points in Euler coordinates would decrease noticeably. I used this fact in 1961 in a theoretical work [12] to prove that my scheme does approximate (in Euler coordinates) the gas-dynamic equations in a sense of conservation laws (in the one-dimensional case). Starting this work, I hoped to prove the convergence to the exact solution as well, but I failed to that. Even the proven order of approximation turned out to be $2/3$—less than one. Just a reminder: formally my scheme has the first order of approximation on the basis of the first differential approximation. I should also note that apparently the actual order of approximation is higher than $2/3$. Most likely, using Glimm's estimates for the variation of the solution [7], one should be able to prove that this order is equal to one, just as it looks. Unfortunately, I haven't studied this issue any further. In the end of the fifties, I was more interested in the question of the precision of the approximated solutions (i.e., what power of the mesh width approximates the error between the calculated solution and the exact one) rather than the issue of the approximation of the equations. The obtained estimations for the approximation order played only an introductory role in the theoretical investigations, which I never finished. However, in 1957–1958 together with V. S. Rjabenkii, I conducted an experimental study of the convergence of the approximate solutions obtained with my scheme to the exact ones. Observing the results, I realized that the convergence should be understood in a "weak" rather than "strong" sense, so that large deviations in a few points would not be important. These deviations usually result from a collision of two shocks or a reflection of a shock from a contact.

During our discussions of this subject, Rjabenkii suggested a trick that reduces the investigation of weak convergence to the study of strong convergence for *one-dimensional problems.* One should look at the integrals (or even multiple integrals) with respect to a spatial coordinate, of the variables obeying the conservation laws, rather than at these variables themselves. We hoped to be able to demonstrate a first order of weak convergence, in agreement with the formal order of approximation. However, to our surprise, the effective order of approximation proved to be less than one for flows with centered expansion waves or large gradients in smooth domains bounded by strong discontinuities.

During this time we were so busy that we did not have enough time to put our conclusions in the form of a detailed article, one of the contributing facts being that the results were unexpected and very unpleasant (at least for me). I limited myself just to a brief report at one of the scientific conferences held at Moscow University. In my view, nobody paid any attention to it. Only N. S. Bahvalov got interested and performed a theoretical study of the convergence speed as $\varepsilon \to 0$ for Burgers' equation

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

which gave an estimate of the order of the error of $\varepsilon|\ln \varepsilon|$. All my attempts to attract attention of the numerical people (who performed the calculations) and engineers (who used the results) to these facts did not have any success.

The major research effort of my group, which included A. V. Zabrodin, K. A. Bagrinovskii, G. B. Alalikin, and me, at that time was focused on the preparation for the

two-dimensional calculations, which I will tell about below. Thus, the question of whether the first-order scheme gives a first-order convergence rate, or more precisely—what is this order—remained unsolved.

I know that in later works of B. van Leer [42], P. R. Woodward and P. Collela [43], P. D. Lax [35], A. Harten [34], and many others, schemes with the effective order of approximation higher than the first were suggested. When these works appeared I had already left the Institute of Applied Mathematics in Moscow, moved to Novosibirsk and was working on different projects. The most significant of these projects involved problems which had arisen in Moscow and required thorough theoretical research. These were questions about the precise mathematical formulation of conservation laws and thermodynamical equalities, about energy integrals for hyperbolic problems, about the mathematically well-posed formulation of the plasticity equations, and about the formulation of computational problems in numerical linear algebra. As I have mentioned earlier, the last question surprisingly enough resulted from the construction of two-dimensional difference schemes. Researching all these numerous and interesting questions (see [17, 14]) diverted me from the investigation of finite-difference methods and did not allow me to gain a deep perception of the modern numerical schemes for gas-dynamics, some of which are known as "second-order Godunov's methods." In all confidence I can state that I cannot consider myself to be their author. It is possible that their real authors were inspired by my suggestion to use the exact solutions of elementary problems as building blocks for the scheme. I have the pleasant responsibility to cordially thank them all for the attention they paid to my work.

Very recently, just about two years ago, I found out that V. V. Ostapenko (from the Novosibirsk Institute for Hydrodynamics, named after M. A. Lavrentiev) is actively working on the problem of the effective precision of hydrodynamic difference schemes, using asymptotic expansions. I suggested to him that instead of horrendous analytical constructions, he should carry out an experimental investigation following the pattern we have developed with Rjabenkii in 1957–1958. I hoped that he would also repeat our experiments, and these would be finally described in detail in the literature. However, Ostapenko concentrated his attention on a more modern Lax–Harten scheme [34], for which he also discovered a difference between formal order of approximation and effective order of precision (order of convergence). At the same time, from the experimental results of Ostapenko it apparently follows that the weak convergence rate for the Lax–Harten scheme is not lower than first, i.e., higher than for my original scheme.

From my point of view, it would be very interesting today to perform experimental investigation of precision for all practical numerical methods. It would be particularly interesting for the two- and three-dimensional problems, for which experimental techniques are yet to be developed.

Finally I note that the transformation of my numerical scheme into a computer program occurred with active help of K. A. Semendjaev, whose experience most certainly contributed to our success.

3. TWO-DIMENSIONAL PROBLEMS AND MOVING GRIDS

Even before the work on one-dimensional methods was finished, I had started to think about two-dimensional versions of my algorithm. The first attempts to solve two-dimensional problems were made in Stekhlov's institute and later in our institute by K. I. Babenko and

I. M. Gelfand. Arising difficulties were discussed at seminars with participation of M. K. Keldish. These discussions proved to be very fruitful. For example, schemes explicit in one variable and implicit in another ("sausages") first appeared at these meetings. Later, the first version of a computationally effective method for block-diagonal systems (a generalization of what is known in English as the Thomas algorithm) was put forward by Keldish and investigated by K. I. Babenko and N. N. Chentsov. For a long time a presentation made by O. V. Lokutsievskii about the instability of a contact discontinuity (based on a chapter from Rayleigh's book "Theory of Sound") was discussed. It can be shown that the time evolution of a contact discontinuity is governed by equations for which a Cauchy problem is ill-posed in the Hadamard sense (not just unstable). Ill-posedness is manifested in the fact that the amplitude of short waves grows unlimitedly fast. Instability is a similar phenomenon; however, the characteristic time for the amplitude growth is bounded for all wavelengths. It was assumed that the processes governed by ill-posed equations cannot be solved by numerical methods. Everybody expected the schemes to become unstable. We talked about some artificially imposed regularization of the boundary conditions on the contacts, but I do not remember if any realistic suggestion for this regularization was ever made.

As a result of these discussions, I developed an intense fear of flows in which contact discontinuities were a possibility. However, at that time there was a large interest in problems which were almost one-dimensional, e.g., problems with slightly curved shocks and sound waves and close-to-planar contact discontinuities. It occurred to me that for this class of problems a simple generalization of my scheme could be used, and I started to work on this modification. My research was approved by Keldish and Gelfand. K. A. Bagrinovskii and G. B. Alalikin took an active part in the development of the first variant of the algorithm. Later, A. V. Zabrodin joined our team. The program was again written by V. V. Lucikovich and G. N. Novozhilova. As usually happens, when our two-dimensional codes were ready, the pressure from engineers pushed us to more and more complicated problems. This required further refinement and improvement of the codes and numerical methods. Busy with all the tailoring, we completely forgot about the major danger—the ill-posedness of the contact discontinuity, and as far as I know, it never appeared as a problem.

I am still perplexed that we never had any problems with regard to the ill-posedness of contacts. Apparently, the difference equations applied to the calculations of the motion of discontinuities provide some kind of regularization. If this is true, one should be concerned with the mechanism of this regularization, which is unknown and, thus, might have some undesired side-effects.

From my point of view, *a detailed study of algorithms used in calculations of contact discontinuities is still an important task.* I am sure that even now a number of new phenomena are waiting to be discovered.

One should note that calculations with moving grids, in which the movement of the discontinuities induces the movement of the nodes of a two- or three-dimensional grid, have not yet been thoroughly investigated, neither theoretically nor experimentally. I am certain that the feed-back effects of the grid motion on the motion of the wave are still unknown.

The first question we faced in our attempts to generalize our method for two dimensions was how to find a solution of the two-dimensional Riemann problem with arbitrary initial conditions. Rectangular cells can border not only along the sides but also in the corners, where four different cells touch each other. In order for a two-dimensional method

to be absolutely similar to the one-dimensional one we needed an analytical solution of the gas-dynamic equations with four initial discontinuities coming together in a single point. Naturally, we did not have these solutions at that time and they are still unknown (for general initial conditions). At this point, a roguish suggestion was made which was to use only the solutions of a classical Riemann problem involving only planar waves. Thus, the interaction of the four cells with a common vertex was neglected altogether. This removed a nice physical interpretation underlying the construction of the one-dimensional scheme. Quite naturally, there were many arguments during the discussion of this hardly justifiable suggestion. Eventually, we decided to test the method by a calculation of a shock, or even an acoustic wave, traveling along the diagonal of the grid. Meanwhile, L. V. Brushlinkii, on the advise of Gelfand, carried out the analytical solution for an acoustic wave propagating in stationary media, which took into account the interaction of the cells sharing a common vertex. He used Sobolev's method of functionally invariant solutions. His solution was implemented in a scheme completely analogous to the one-dimensional one. After that, we compared the calculations of diagonally propagating waves using Brushlinkii's scheme to our simple method. To our surprise and pleasure there were no significant differences. Afterwards, only the simpler model was used. A large effort went into the development of a stability criterion to limit the time step for a prescribed spatial step. Originally, using a Fourier method, Alalikin, Bagrinovskii, and I arrived at a cubic characteristic equation, from which we obtained only the necessary stability conditions. Later, together with Bagrinovskii, we were able to obtain sufficient stability conditions as well. In doing so, we considered a two-dimensional method as a certain averaging of one-dimensional calculations; this technique is now known as "splitting." This work [2] was published in 1957 at a time when our two-dimensional code had already been used for a number of rather intricate calculations.

The idea to use "splitting" appeared while we were investigating implicit schemes for the two-dimensional heat equation. Similar schemes were proposed later by J. Douglas and co-authors. However, at the time, we rejected using splitting methods for solving two-dimensional parabolic equations.

The toughest test for gas dynamical schemes was the calculation of a discontinuous solution. Thus, I decided to test my new scheme for the heat equation $u_t = u_{xx} + u_{yy}$ on the least smooth case. I started to investigate the spreading of an initial heat pulse released in a single computational cell. In other words, I had been trying to model a solution which after some time should be close to

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

At the least, the level contours of the solution should be convex curves—nearly circles.

To my great surprise, in the calculation, with the Courant number

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

these contours turned out to be cross-like, at least for the first few steps. The results heavily discouraged me from using splitting methods for the heat equation. Nevertheless, this research suggested the use of splitting for proving the stability of gas dynamical schemes, and also for the organization of a computer program.

The first two-dimensional program was written in such a way that, in subsequent steps, it used fluxes calculated with the one-dimensional method in alternating grid directions. It did not cause any troubles, but later we quit using directional splitting in explicit schemes on the suggestion of Lucikovich, who claimed that he could make the codes simpler and more efficient without splitting. Before that, we were sure of the opposite, that splitting would make our codes faster.

I have already said that, for two-dimensional problems, we had to switch from Lagrange to Euler coordinates. Then, in order to connect the grids with the moving boundaries, we had to make the grids move as well. This also allowed us to consider shock waves as a special type of boundary. It turned out to be very useful in the above-mentioned calculation of the flow past a sphere [31].

I should mention that in the first versions of our two-dimensional methods we were extremely careful about the construction of the grid cells and wrote the difference schemes for conservation laws very pedantically. For example, we used the arcs of logarithmic spirals as the boundaries of the cells and the exact analytical expressions for the integrals over the cells bounded by these spirals. It was only a few years later when we allowed ourselves to introduce some simplifications. The hard work of evaluating the numerous required integrals was performed by K. A. Bagrinovskii and A. V. Zabrodin.

Even in one-dimensional calculations using Lagrangean coordinates we were trying to improve the accuracy by tracing the motion of the strongest shock waves. In order not to smear out the waves, their positions were marked and the cells where these waves were located were split into two parts. Hugoniot relations were used to calculate the motion of the waves. When we started to use the Euler coordinates the need to distinguish between the two types of the boundaries (shocks and contacts) disappeared. This simplified the logistics of the algorithms and allowed us to introduce a new type of boundary, with a prescribed initial position and motion, which did not affect the flow in any way. These boundaries were suggested by Zabrodin and were referred to as “Euler boundaries.”

The coordinates of the grid nodes inside a domain surrounded by boundaries of different types were calculated by a simple interpolation from the boundaries. Of course, the movement of the boundaries at each step caused the motion of the grid nodes. Programs with this kind of grid structure allowed us to achieve better accuracy, not through the improvement of the difference schemes, but just because the grids were adapted to the solution structure and the strong discontinuities were carefully traced and not smeared out. During the work with these types of codes I got an impetus to replace the interpolation for the internal grid nodes by a solution of a system of differential equations which described a mapping from the domain in question onto some standard domain as a rectangle. We started to study this problem with G. P. Prokopov and spent seven years (1961–1968) before the first acceptable results emerged [13, 19, 22].

I am still concerned with the type of mapping that should be used for the grid generation, although I quit working on difference schemes a very long time ago [28].

From the very start of this work, we postulated that the mapping should be a solution of an elliptic system of equations. Our main effort was concentrated on solving these equations effectively. We decided to use a variational approach utilizing the finite-element method. However, we did not dare to test this approach by calculating the grid for a real gas-dynamic problem with moving boundaries, since solving an elliptic problem at each time step would be costly. First, it was decided to use a variational approach in some stationary problem. Specifically, we applied our developments to the calculation of critical parameters of nuclear

reactors [38]. I have mentioned before that it was during this work that my interest in the computational problems of linear algebra was awakened. Later in my career I devoted most of my attention to these types of problems.

Only after success with stationary problems did we dare to build computational grids at every time step by solving elliptic equations. The first more or less general-purpose computer code of this type started to operate in the end of 1968 or in the beginning of 1969. The first problem was applied to provided the basis of a paper [33]. This paper was an expanded version of our presentation at the International Conference on the Physics of Explosion (Novosibirsk, 1969). This work was devoted to the wave generation during welding by explosion and contained the analysis of the experiments performed at the Novosibirsk Institute for Hydrodynamics.

In September 1969, I moved to Novosibirsk and since then have done little work with regard to numerical schemes.

It seems to be worth mentioning that while developing the schemes for two-dimensional calculations we had been simultaneously applying them to one-dimensional problems, trying to get the best possible precision. The extraction as boundaries of contact discontinuities, shock waves and characteristics bounding the rarefaction waves allowed us to segregate the computational domain into subdomains inside of which the solution was supposed to be smooth. Inside these domains we were able to use second-order methods. It is very important that for each rarefaction wave from the moment of its emergence from an arbitrary discontinuity a large number (for example, 50) of grid points was reserved. This provided very high precision and was possible because we used implicit schemes.

I developed the described methods together with I. L. Kireeva and L. A. Pliner, while the logistics of the algorithm were put forward by G. B. Alalikin. He also wrote a general-purpose computer program on the basis of our algorithm. This code was used for a number of high-precision calculations. All these methods were described in our book [1] published in Russian in 1970. I think it passed unnoticed. At the same time, I believe that specialists in computational fluid dynamics even today can find something interesting in it.

I should note that under some pressure from engineers and Semendjaev, parallel to the work on the two-dimensional scheme, I had to work on the method of characteristics as well. I had been trying to make it suitable for computer implementation by reorganizing the information structure. This resulted in the methods of "characteristics layers," in which not the intersections of characteristics were calculated, but rather the coordinates where the characteristics cross the layers $t = \text{const}$. However, when the work was finished and a rather intricate general-purpose program was written, we discovered flaws in the method. The very first tests showed that it failed for calculations with strong rarefaction waves. This was a surprise since we expected the method to perform better in such cases than anything else. A brief report on this failure was published [26]. The failure itself pushed me to the development of a second-order method with discontinuities extracted as boundaries, which is discussed in the above-mentioned book [1].

Wide recognition of the difference scheme for gas dynamics based on the break up of an arbitrary discontinuity started in 1969. This year at the conference in Novosibirsk there were in total three independent presentations related to our scheme. I have already mentioned our report. In addition to that, there was a presentation by M. Ja. Ivnanov and A. N. Kraiko from the Moscow Central Institute for Aircraft Engines (we did not know each other before) and a presentation by T. D. Taylor and B. S. Mason (U.S.A.) about the application of our scheme to

the flow around the return vehicle "Apollo" [36, 41]. Together with our colleagues from the Institute for Aircraft Engines, we later prepared a detailed description of our computational methods and published it as a book which was translated into French [15].

4. CONSERVATION LAWS AND THERMODYNAMICS

Finally, I will briefly discuss one more issue closely related to the concept of generalized solutions of quasi-linear systems of conservation laws. This is another example of research which arose during my work on difference schemes.

As it was mentioned above, mass, momentum, and energy are conserved exactly for the numerical solutions calculated with my scheme. However, the classical (smooth) solutions of gasdynamical equations obey an additional conservation law—that of entropy. Zemplen's theorem states that across a shock wave (discontinuity in the solution) entropy increases. In the theory of quasi-linear equations this statement is very important in the definition of generalized solutions. It outlaws the flows which are in agreement with the conservation of mass, momentum, and energy, but for which the entropy is decreasing for a certain mass of gas. In my original scheme the entropy was automatically nondecreasing because the update method used the physical solutions of the Riemann problem, which comply with the entropy principle. Each time step was finished by averaging the state variables over the cells, and one can easily show that this process can only increase the entropy.

Naturally, I got interested in the class of quasi-linear systems of equations for n unknowns which satisfy $n+1$ conservation laws. While pondering these systems in general, I noticed that all the nonlinear relations in the equations of hydrodynamics are completely determined by a single function—the thermodynamic potential $E(V, S)$. Gelfand had mentioned an important role of the inequalities $E_S > 0$ and $E_{VV}E_{SS} - E_{VS}^2 > 0$ in his lectures on the theory of quasi-linear equations. He gave these lectures at Moscow University, and later his lecture notes were published as a book [6]. These inequalities are used in thermodynamics for gases and liquids when V and S are far from the phase-transition values. As a problem, Gelfand suggested proving that these inequalities ensure the well-posedness of the wave propagation problem in the acoustic approximation for heat-conducting gases. Influenced by that problem, I got the idea that a similar consideration about well-posedness or about stability (at least in the case of a finite number of degrees of freedom) can be based on the famous theorem of thermodynamics about the existence of a universal integrating multiplier $1/T$ for $dE + pdV$. This theorem underlies the definition of the entropy as $dS = (1/T)(dE + pdV)$. After a few months of intensive work, I was able to justify this hypothesis [9]. As a by-product I proved that the stability which makes impossible a perpetual motion machine of the second type always results from the existence of some integral, which is dissipated by heat-conduction. In the limit of small oscillations (i.e., when the evolution of the system is described by a linear system of equations) this integral turns out to be a quadratic form with a symmetric and positive-definite matrix of coefficients. The symmetry of the matrix leads to the equalities which are needed to derive the existence of the universal integrating multiplier. My paper [9] (see also Section 22 of the book [14]) had the blueprints of a mechanism that would have been the perpetual engine of the second type in a world without the universal integrating multiplier.

After this work [9], trying to understand the reason why a system of three equations would have an "extra" fourth conservation law, it was very natural to write the hydrodynamic

equations in Lagrangean coordinates (applicable for the classical smooth solutions),

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

and to derive the fourth conservation law as their linear combination

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

This equation shows that the four conservation laws are linearly dependent. Then, of course, any of the four conservation laws can be composed of the other three. For instance, conservation of entropy $\frac{\partial S}{\partial t} = 0$ may be expressed as a linear combination of conservation of specific volume

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

conservation of momentum

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

and conservation of energy as

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

The last equality uses 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 rewrite this relation as

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

Now we introduce the notation

$$L = S - \frac{1}{E_S}\left(E + \frac{u^2}{2}\right) + \frac{VE_V}{E_S} + \frac{u^2}{2E_S} = \frac{1}{E_S}[SE_S + VE_V - E],$$
$$q_1 = \frac{E_V}{E_S}, \qquad q_2 = \frac{u}{E_S}, \qquad q_3 = -\frac{1}{E_S} = -\frac{1}{T}.$$

Finally, we can relate the derivatives L_{q_i} to the hydrodynamical quantities

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

The relation between differentials $dS, dV, du, d(E + u^2/2)$ takes the beautiful form of the Legendre transformation from the theory of convex functions,

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

It is convenient to introduce one more function

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

Then

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

This allows one to write the hydrodynamic equations as

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

They consist of three conservation laws, and the additional fourth conservation law

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

coincides with the conservation of entropy $\frac{\partial S}{\partial t} = 0$. After this, it was not too difficult to rewrite a number of other classical equations of mathematical physics (even multi-dimensional) in a standard form

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

I succeeded in writing out in a similar form the gasdynamic equations in Euler coordinates as well. I was very glad to be able to show that if the generating "thermodynamic potential" is convex then these equations can be cast into a form of a symmetric hyperbolic system

(in the Friedrichs sense)

$$L_{q_i q_k} \frac{\partial q_k}{\partial t} + L^j_{q_i q_k} \frac{\partial q_k}{\partial x_j} = 0.$$

The matrix multiplying the time-derivative is positive-definite. K. O. Friedrichs showed that for these equations the Cauchy problem is well-posed if the initial conditions are smooth enough.

In such a way, my hopes to show the connection between well-posedness and the laws of thermodynamics started to take a solid form.

I have described my achievements in a paper, submitted to *Uspekhi Matematicheskikh Nauk*. It was not published though, since the referee denied its mathematical content.

Soon after this I experienced yet another unpleasant twist of fate. I decided to add a small dissipation to the above form of the equations to investigate the structure of discontinuities. I was interested to know if the viscosity smears discontinuities only over a thin region, and if the limiting solutions for vanishing viscosity do not depend on the particular form of the dissipative term. Considering steadily propagating waves $q_i = q_i(\xi)$, $\xi = (x - wt)/\varepsilon$ for the 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 was able to obtain a nice geometrical interpretation for the ordinary differential equations, satisfied by $q(\xi)$. This interpretation helped me to construct a system of hyperbolic conservation laws for which the admissible discontinuous solutions do depend on the form of the dissipation terms (while still satisfying the entropy condition). In a real physical problem the dissipation processes can be very different from those in the numerical calculation. Different numerical schemes have different dissipation properties. Soon afterwards, V. F. Diachenko suggested an example in which different difference approximations resulted in very dissimilar numerical solutions [3].

At that time I was very depressed because my hope to justify all the hypotheses underlying my difference scheme collapsed. My paper with the description of the above-mentioned counter-example was communicated to *Dokladi AN SSSR* by I. G. Petrovskii [10, 11]. Even before the article was published I presented it at a seminar where R. Courant and P. D. Lax were present. It was during their first visit to Moscow.

Later, in Novosibirsk, together with my colleagues I continued the investigation of the conservation laws and their relation to thermodynamics. An overview of a large part of this research can be found in the presentation [17], which I made in 1986 in St.-Etienne, France, at the conference on hyperbolic equations. One should also note the important contributions to this subject [5, 4] made by Lax and Friedrichs. Recently this work was continued even further and became the subject of the presentations by E. I. Romenskii and myself at Lisbon [23], Lake Tahoe [24], and Paris [25]. Another work of ours (together with T. Yu. Mihailova) is devoted to a similar issue [29]. In [25, 29] an unexpected connection between the formally overdetermined systems of conservation laws of mathematical physics and the theory of representation of the rotation group has been shown.

Finally, I mention a recent work [40] in which estimates of the entropy growth for the systems introduced above were made. The author succeeded in relating these estimates to the variation of the solution. I found the method for determining this variation suggested in

the article to be very promising. For this method it makes no difference if the problem in question is one- or multi-dimensional.

5. CONCLUSION

In these notes I have tried to recount the intensive work in the field of numerical hydrodynamics in which I took part; this work resulted in the development of "Godunov's scheme."

I want to emphasize that during that period I was influenced by the whole scientific community I was immersed in. Of course, there were many other research groups working on different approaches to numerical hydrodynamics. Some of these groups belonged to the institute where I worked. The more famous scientists associated with other computational fluid mechanics groups of that time are K. I. Babenko, V. V. Rusanov, I. M. Gelfand, V. F. Diachenko, A. A. Samarskii, N. N. Janenko, B. L. Rozhdestvenskii, and others. I did not try to describe the whole history of the subject, but rather, to tell about some of the research activity in which I took part myself.

I greatly benefited from numerous discussions with prominent 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. I should mention that the comments of physicists were often very fault-finding. They stimulated the detailed analysis of the causes of numerical effects and often led to modifications and improvements of the method. The specific problem for stationary flow past a body was suggested to me by G. I. Petrov.

I also wanted to show how a whole series of important scientific questions appeared during the initial stage of the development of computational fluid dynamics. Many of these questions are still unresolved.

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