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Methods for the Localization of Singularities in Numerical Solutions of Gas Dynamics Problems

气体动力学问题数值解中奇异点局部化方法〔英〕

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Preface

As a result of the numerical simulation of multidimensional gas dynamics problems on a computer, the output information is obtained in the form of immense arrays of numerical data. In this connection, there arises the problem of extracting the actually needed information from these arrays; in other words, it is necessary to solve the problem of information compression. In particular, the numerical solution of gas dynamics problems often aims at the information on the solution singularities—the shock waves, contact interfaces, slip lines, etc. Our book is devoted to the development and investigation of accuracy of the algorithms for the localization of such singularities. In addition, the questions of development of the algorithms for the classification of singularities into several types (on the basis of shock-capturing numerical solutions of two-dimensional gas dynamics problems) are considered for the first time in the monographic literature. For this purpose, some ideas and methods of the modern theory of digital-image processing and of the pattern recognition theory are used. The information obtained at the output of the systems of the singularities classification presented in this book is rich in content, because it contains both physical and geometrical characteristics of recognized objects. Therefore, such "intellectual" systems of information extraction may be used in the expert systems of automated design of aerodynamic bodies which meet some optimality requirements. This is, in our opinion, very attractive from the point of view of applications.

The methods of differential approximation, variational calculus, and numerical optimization have been used in the studies of accuracy of the well-known algorithms for the localization of singularities, as well as the new algorithms proposed by the present authors.

We have aimed at a balanced presentation of the material, therefore, the applications of developed algorithms of the singularities localization to the analysis of various two-dimensional fluid mechanics problems have been included in the book along with the theoretical results. In particular, we have considered problems of high-velocity impact, transonic flow around an airfoil, hypersonic flow around a nonconvex body, etc.

We express our gratitude to the research workers of the Department for Numerical Methods of Continuum Mechanics of the Computing Center of the U.S.S.R. Academy of Sciences, Siberian Branch, and to professional

colleagues from the Institute of Theoretical and Applied Mechanics of the U.S.S.R. Academy of Sciences, Siberian Branch, in whose collectives the work had been discussed. Our opinions and points of view were also affected by the interaction with collectives headed by A.N. Tikhonov, L.V. Ovsyannikov. The discussions with Yu.A. Berezin, Yu.M. Davydov, V.M. Fomin, A.N. Konovalov, B.G. Kuznetsov, V.A. Novikov, V.V. Pikalov, N.G. Preobrazhenskii, B.L. Roždestvenskii, V.V. Rusanov, Yu.I. Shokin, A.F. Voyevodin, Yu.S. Zavyalov were especially useful to us. We are very grateful to the editor of the English language edition of this book, V.V. Rusanov, for his careful editing of the manuscript.

We also express our thanks to Professor K.G. Roesner from Darmstadt, F.R.G., who immediately recommended our book to Springer-Verlag in Heidelberg, having read the Russian edition of the book. We are grateful to Professor W. Beiglböck, the editor of the Springer Series in Computational Physics, for allowing us to publish in this series, and to T.A. Alexandrova for typing the manuscript.

Contents

CHAPTER 1

Introduction and Necessary Notions from the Theory of Difference Schemes for Gas Dynamics Problems

The use of electronic computers in numerical simulations of gas flows with singularities started practically immediately after the first such computers had appeared in the 1940s [1.1], [1.2]. Presently, a wide application of computers for the solution of various fluid dynamics problems has become possible, owing to the development of powerful computers and efficient numerical methods—and the corresponding field of science has been termed "computational fluid dynamics" [1.3], [1.4].

In the course of mathematical modeling of many fluid dynamics problems one often has to deal with the solutions containing singularities of various types. For example, in the problems of inviscid compressible gas dynamics there are singularities of shock wave and contact discontinuity type [1.5], in the filtration problems there are saturation fronts [1.6]. In combustion problems one has to deal with flame fronts [1.7], in turbulence theory with coherent structures [1.8], in meteorology problems with atmospheric fronts [1.9], in magnetohydrodynamics with magnetohydrodynamic shock waves [1.10], [1.11], etc. At present, finite-difference shock-capturing schemes are widely used for the numerical investigation of such problems. In the numerical solutions obtained with the aid of such schemes the discontinuities are approximated by some transition regions, the size of which (in the direction of a normal to the discontinuity surface) is usually equal to several intervals of a spatial computing mesh. As a result of this it proves difficult to effectively use and interpret the numerical data obtained and, in addition, there arises the problem of increasing the accuracy of difference solutions in the neighborhood of discontinuities. In particular, a research worker dealing with shocked gas flows is in many cases interested primarily in the information on shock surfaces: their disposition, shape, propagation speed, etc.

In connection with the foregoing there exists a need, in the development and foundation of specialized algorithms, to process the numerical results of solving fluid dynamics problems which are intended for the localization of discontinuity surfaces in a flow and for their classification into several types (shock waves, contact interfaces, etc.).

A problem of development of the singularities localization techniques on the basis of finite-difference solutions is closely related to increases in the accuracy of numerical solutions in the vicinity of discontinuities. Localization of strong discontinuities is substantially facilitated if one uses, in computations, a finite-difference method which enables one to reduce the width of a zone of discontinuity "smearing" to the size of one mesh interval. In this case it is possible to use, for shock localization, the already existing simplest procedures, for example, by maximum coalescence of isolines (for example, isochors) or by maximum gradients of any of the functions sought which undergo a discontinuity.

The structure of shock localization algorithms will also be affected by a further increase in the performance of computers. For example, a considerable increase in the computer core memory, as well as the use of parallel processors, enables one to use substantially finer meshes. Then the accuracy of determining the location of a discontinuity within the zone of its "smearing" is not so important as in the case of crude meshes, and it will then be possible to successfully apply the simplest procedures for the numerical shock localization. On the other hand, a manual processing of the results (and even a simple survey of them) becomes difficult with the increase in the number of grid points. Computer methods of processing can substantially aid the researcher in the interpretation of numerical results in this case. They also facilitate substantially the computer generation of pictures of temporal evolution of various singularities in cases when such pictures are of primary importance. If the solution accuracy in the neighborhood of discontinuities, which is achieved in the case of using a specific difference scheme, is insufficient, then the informaton on the singularities locaton may be incorporated directly into a computational algorithm to achieve an increase in the accuracy of computation (see Chapters 2, 3, and 6).

In addition, the localization of discontinuities, in particular, the ones arising in the process of computation, gives an opportunity of an active control of this process which may include, for example, the alteration of some boundary conditions, a switch to another construction of a difference grid or to another difference scheme, etc.

Mathematical models of the above-listed various problems of fluid dynamics are characterized by different levels of complexity. In our monograph we analyze a wide spectrum of algorithms for the localization and classification of strong discontinuities in the numerical solutions of inviscid compressible non-heat-conducting gas dynamics. This has been done for two reasons. First, the flows with singularities of different types (being different from the ones known in gas dynamics) are at present treated in much the same way as the gas-dynamical shocked flows (see, for example, [1.7], [1.12], [1.13]). Second, the results of the investigation of various algorithms for the strong discontinuities localization (presented in Chapters 2–7) were obtained by the present authors only for gas dynamics problems described by the Euler equations. Taking the above into account, the domain of applicability of the methods for the localization and classification of singularities on the basis of shock-capturing numerical solutions presented below goes beyond the scope of inviscid gas dynamics problems. The essence of a general approach (presented in our book) to the development and investigation of shock localization methods based on shock-capturing computations is in the maximal use of information on the structure of a finite-difference solution in the zone of "smearing" of a strong discontinuity, while constructing the algorithms for locating a true discontinuity within a zone of its numerical smearing. Aiming at brevity of presentation, we emphasize our own results; therefore, other algorithms of the singularities localization which are known in the literature are mentioned only briefly at the beginning of Chapters 2 and 4. We make no claim to completeness in the list of references where the localization algorithms developed by other authors are presented, although we hope that we have presented in this list the basic ideas and trends in the construction of the above algorithms.

The methods of the singularities localization presented in Chapters 2–6 can be united into one big group of methods whose realization is related substantially to the use of *a priori* information on the orientation of shock surfaces with respect to the axes of spatial coordinates. However, in some cases, such informaton is absent. There are, for example, such problems, the investigation of which is difficult to carry out by other techniques (for example, by experimental techniques), and then mathematical modeling becomes the only method of studying such complicated phenomena or processes [1.14]. The methods for the localization and classification of singularities which are presented in Chapter 7 may prove to be very useful in the analysis of computational results of such problems. These methods do not require for their implementation any *a priori* information on the presence or absence of singularities in the problem under consideration, as well as on their approximate orientation with respect to the spatial coordinate axes. The methods of Chapter 7 use substantially the ideas and algorithms of the digital-image processing theory and the theory of pattern recognition, and are very versatile and universal, and which is shown in a number of examples. Since the data obtained (which is presented in Chapter 7) at the output of a system of extraction of information from the results of two-dimensional gas-dynamical computations is rich in content—it contains both physical and geometrical characteristics of recognized objects—it can be used for controlling the process of the numerical solution of the basic problem as well as for decision-making in the expert systems of aerodynamic automatic design [1.15], [1.16].

Results of investigation of the accuracy of methods for the localization of singularities are illustrated by numerical computations of model problems having exact solutions. In addition, there are demonstrated examples of those complicated fluid mechanics problems, in the analysis of which the developed localization algorithms have been used. These are the high-velocity impact problems, a transonic flow around an airfoil, supersonic flows in annular nozzles and jets, hypersonic flow around a nonconvex body, interaction of jets with obstacles, etc.

This monograph represents the first systematic presentation of the results of accuracy analysis of the methods for the localization of singularities on the basis of the shock-capturing computation of gas dynamics problems. A number of new results obtained by the present authors is presented for the first time.

1.1. Original Equations. Jump Conditions in the Case of One-Dimensional Gas Flow

1.1.1. Divergence and Nondivergence Form of Equations

The system of differential equations governing the plane one-dimensional flow of an inviscid compressible non-heat-conducting gas, which depends on time t and on one Cartesian coordinate x, has the following divergence form [1.17], [1.18]:

$$\partial\rho/\partial t + \partial\rho u/\partial x = 0; \tag{1.1}$$

$$\partial\rho u/\partial t + \partial(p + \rho u^2)/\partial x = 0; \tag{1.2}$$

$$\partial\rho(\varepsilon + u^2/2)/\partial t + \partial[\rho u(\varepsilon + u^2/2) + pu]/\partial x = 0. \tag{1.3}$$

Here ρ is the density, p is the pressure, ε is the internal energy per unit mass of the gas, and u is the velocity in the direction of the x-axis. The four functions ρ, u, p, ε sought enter into the system (1.1)–(1.3). Therefore, one more equation is necessary to complete this system. As is known, among the thermodynamical quantities describing the gas state only the two quantities are independent, the remaining quantities can be expressed in terms of two chosen independent functions with the aid of an equation of state [1.18]. In particular, let the equations of state be given in the form

$$p = G(V, S), \qquad T = T(V, S), \tag{1.4}$$

where V is the specific volume, $V = 1/\rho$, S is the entropy, and T is the gas temperature. Then the specific internal energy ε may be calculated as a function of the variables V, S, with the aid of a thermodynamical identity $d\varepsilon + p\,dV = T\,dS$. Knowing the dependencies of the quantities p and ε on V and S, we can compute the pressure p as a function of ρ, ε:

$$p = F(\rho, \varepsilon). \tag{1.5}$$

Thus, in the case when the equation of state can be given in the form (1.5), the system of equations (1.1)–(1.3) is closed without using the entropy S. In the following we shall assume the presence of a dependency (1.5) or of a dependency

$$\varepsilon = f(p, \rho). \tag{1.6}$$

Of course, the functions f and F are such that the identity

$$p \equiv F(\rho, f(p, \rho)) \tag{1.7}$$

takes place. The ideal gas equation of state

$$p = (\gamma - 1)\rho\varepsilon \tag{1.8}$$

is one of the simplest equations of state, where the quantity γ is the ratio of specific heat, usually $\gamma = \text{const} > 1$.

In the following we shall often use a vector notation of the system (1.1)–(1.3). Introduce the column vectors

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix}, \qquad \boldsymbol{\varphi}(\mathbf{u}) = \begin{pmatrix} \rho u \\ p + \rho u^2 \\ pu + \rho u E \end{pmatrix}, \tag{1.9}$$

where

$$E = \varepsilon + u^2/2, \tag{1.10}$$

that is, E is the total energy per unit mass of the gas. Then the system (1.1)–(1.3) may be written in the form

$$\partial \mathbf{u}/\partial t + \partial \boldsymbol{\varphi}(\mathbf{u})/\partial x = 0. \tag{1.11}$$

The system (1.11) is the divergence, or conservative, form of the Euler equations. We shall also need a nondivergence form of the system (1.1)–(1.3). Set

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, \qquad \boldsymbol{\varphi} = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{pmatrix},$$

where

$$u_1 \equiv \rho, \qquad u_2 \equiv \rho u, \qquad u_3 \equiv \rho E;$$

$$\begin{aligned} \varphi_1 &= \rho u = u_2, \\ \varphi_2 &= p + \rho u^2 = F(u_1, (u_3/u_1) - 0.5(u_2/u_1)^2) + u_2^2/u_1, \\ \varphi_3 &= F(u_1, u_3/u_1 - 0.5(u_2/u_1)^2)(u_2/u_1) + u_2 u_3/u_1, \end{aligned} \tag{1.12}$$

$F(\rho, \varepsilon)$ is the function entering the equation of state (1.5). Then the elements of the Jacobi matrix

$$A = \partial \boldsymbol{\varphi}/\partial \mathbf{u} \tag{1.13}$$

are determined by the formulas $a_{lm} = \partial \varphi_l/\partial u_m$. In the case when the equation of state (1.5) is employed to complete the system (1.1)–(1.3), the elements a_{lm} have the following expressions (see, for example, [1.19])

$$\begin{aligned} &a_{11} = 0; && a_{12} = 1; && a_{13} = 0; \\ &a_{21} = \theta + rz - u^2; && a_{22} = u(2 - z); && a_{23} = z; \\ &a_{31} = -u(E + m - \theta - rz); && a_{32} = E + m - u^2 z; && a_{33} = uz_1. \end{aligned} \tag{1.14}$$

In formulas (! 14) $r = u^2 - E$, $z = (1/\rho)\,\partial p/\partial\varepsilon$, $z_1 = 1 + z$, $\theta = \partial p/\partial\rho$, and $m = p/\rho$. With the use of the matrix A (1.13) the nondivergence form of the system (1.11) may obviously be written as

$$\partial\mathbf{u}/\partial t + A(\mathbf{u})\,\partial\mathbf{u}/\partial x = 0. \tag{1.15}$$

As is known, the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of the matrix A have the form

$$\lambda_1 = u - c, \qquad \lambda_2 = u, \qquad \lambda_3 = u + c, \tag{1.16}$$

where c is the adiabatic speed of sound. In the case of the equation of state (1.5) the square of the speed of sound is calculated by the formula

$$c^2 = (p/\rho^2)\,\partial F/\partial\varepsilon + \partial F/\partial\rho.$$

Thus, if the function $F(\rho, \varepsilon)$ in the equation of state (1.5) satisfies the inequality

$$(p/\rho^2)\,\partial F/\partial\varepsilon + \partial F/\partial\rho > 0, \tag{1.17}$$

then the equation system (1.15) is of hyperbolic type. It is assumed in the following that the equations of state employed satisfy the inequality (1.17). The matrix A whose elements are determir^d by formulas (1.14) also possesses the following property [1.18]:

$$\begin{aligned} (A - uI)^{2k+1} &= c^{2k}(A - uI), \\ (A - uI)^{2k+2} &= c^{2k}(A - uI)^2, \qquad k = 0, 1, 2, \ldots, \end{aligned} \tag{1.18}$$

where I is the unit matrix and c is the speed of sound.

1.1.2. Jump Conditions

Let Ω be an arbitrary subdomain with the boundary Γ in the (x, t)-plane which is in the domain of definition of the system (1.11) solution. Then the integral conservation laws for the system (1.11) have the form

$$\oint_\Gamma \mathbf{u}\,dx - \boldsymbol{\varphi}(\mathbf{u})\,dt = 0. \tag{1.19}$$

Unlike the system (1.1)–(1.3), the relationships (1.19) are also valid for discontinuous solutions. Let us derive the conditions which are to be satisfied along the discontinuity lines of the solutions of gas dynamics equations as consequences of the integral conservation laws. Let $x = x_s(t)$ be the equation of one of the lines of the jump in hydrodynamic quantities, and let the function $f(x, t)$ undergo a jump across the line $x = x_s(t)$. Denote by

$$\begin{gathered} f_1(t) = f(x_s(t) - 0, t); \qquad f_2(t) = f(x_s(t) + 0, t); \\ [f] = f_2(t) - f_1(t). \end{gathered} \tag{1.20}$$

Let the discontinuity propagate at a speed $dx_s/dt = D$. Consider in the (x, t)-

plane a closed contour, two lines of which adhere with an infinite proximity to some segment of the discontinuity line $x_s(t)$. It follows from the conservation laws written for this contour that along the discontinuity line

$$\int ([\mathbf{u}]D - [\boldsymbol{\varphi}(\mathbf{u})])\, dt = 0,$$

where the integrals are taken along any segment of the discontinuity line. By virtue of an arbitrary choice of the integration domain, the relationships

$$[\mathbf{u}]D = [\boldsymbol{\varphi}(\mathbf{u})] \tag{1.21}$$

are valid at each point of a discontinuity which relate the jumps of hydrodynamic quantities across the discontinuity line $x = x_s(t)$ and the speed $D = x_s'(t)$ of the discontinuity line. In the case of the Euler equation system (1.1)–(1.3) equations (1.21) may be written with regard to (1.9), (1.10) as the following three algebraic relations

$$D[\rho] = [\rho u]; \tag{1.22}$$

$$D[\rho u] = [p + \rho u^2]; \tag{1.23}$$

$$D[\rho(\varepsilon + u^2/2)] = [\rho u(\varepsilon + p/\rho + u^2/2)]. \tag{1.24}$$

The relations (1.22)–(1.24) are called the Rankine–Hugoniot conditions. Taking into account the notation (1.20), we can rewrite the Rankine–Hugoniot conditions (1.22)–(1.24) in the form of equations

$$\rho_2(u_2 - D) = \rho_1(u_1 - D) = m; \tag{1.25}$$

$$p_2 + \rho_2(u_2 - D)^2 = p_1 + \rho_1(u_1 - D)^2; \tag{1.26}$$

$$\rho_2(u_2 - D)(\varepsilon_2 + p_2/\rho_2 + (u_2 - D)^2/2)$$
$$= \rho_1(u_1 - D)(\varepsilon_1 + p_1/\rho_1 + (u_1 - D)^2/2). \tag{1.27}$$

If $m(t) = 0$ in equation (1.25), then this kind of discontinuity will be called contact; if $m(t) \neq 0$, then the discontinuity will be called a shock wave. In the case of a contact discontinuity it follows from (1.25) that

$$D = u_1 = u_2 = x_s'(t),$$

that is, the discontinuity line coincides with the particle trajectory. Assuming $u_1 = D$, $u_2 = D$, we obtain from (1.26) that $p_1 = p_2$. The condition (1.27) is satisfied identically at $u_1 = u_2 = D$. Thus, the pressure and the speed of the flow are continuous across a contact discontinuity in the one-dimensional gas flow. In particular, a contact discontinuity may be an interface between two different gases satisfying different equations of state.

In the case of a shock wave, that is, when $m \neq 0$, the Hugoniot adiabatic equation is obtained from (1.25)–(1.27) as an algebraic consequence [1.18]

$$\varepsilon_2 - \varepsilon_1 = (1/2)(p_2 + p_1)(V_1 - V_2), \tag{1.28}$$

where V is the specific volume, $V = 1/\rho$. Zemplén's theorem is valid for stable shock waves. This theorem asserts that the shock wave speed is subsonic with respect to a gas behind the shock front, and is supersonic with respect to a gas before the shock front.

Let the subscript 1 in (1.20) refer to a gas state behind the shock wave front, and let the subscript 2 refer to a state before the front. Then the above assertion (Zemplén's theorem) may be written in the form of the following inequalities:

$$|u_2 - D| > c_2; \qquad |u_1 - D| < c_1. \tag{1.29}$$

1.1.3. Riemann Problem

Concluding this section let us briefly consider the Riemann problem. An arbitrary discontinuity is an initial state of two infinite masses of gas characterized by constant parameters $u_1, p_1, V_1, \varepsilon_1, T_1$ and $u_2, p_2, V_2, \varepsilon_2, T_2$ adjoining along the plane $x = 0$ at the initial time $t = 0$. Here the magnitudes of the discontinuity to the left and right are arbitrary and subject only to the equations of state of the gases which may be different for the neighboring gases.

The determination of the flow arising for $t > 0$ with these initial conditions is called the Riemann problem, or the breakdown-of-discontinuity problem.

If an arbitrary discontinuity is not a contact discontinuity or a shock wave, it decomposes by forming some configuration of stable discontinuities and continuous gas-dynamical flows. All possible configurations of a flow arising in the process of a breakdown of a discontinuity in the gas have been considered in [1.18], [1.20]. Here the configuration A contains a rarefaction wave propagating into the gas "1", and a contact discontinuity and a shock wave propagating into the gas "2" (Figure 1.1(a)). The configuration B contains the shock waves propagating to the left and to the right of the point $x = 0$, and a contact discontinuity (Figure 1.1(b)). In configuraton C there are two rarefaction waves and a contact discontinuity (Figure 1.1(c)). Critical values of the parameters separating one configuraton from another have been derived in [1.18]. Certain flow configurations, which may be called intermediate configurations between the main configurations A, B, C, correspond to these critical values. For example, an intermediate configuration between configurations A and B is the configuration consisting of one shock wave and a contact discontinuity (Figure 1.1(d)). An intermediate configuration between configurations B and C is the configuration consisting of a stagnant contact boundary (Figure 1.1(e)) and a rarefaction wave. In the particular case of configuration C there can occur a separation of the gases "1" and "2" from one another, and then the rarefaction waves are separated by a region of vacuum in which $\rho = p = c = 0$ (Figure 1.1(f)).