On adjoint variables for discontinuous flow

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Abstract

The standard approach to the solution of the adjoint equations stresses the similarity of direct and adjoint equations and implies the use of similar methods for their solution. Nevertheless, the adjoint equations have significant peculiarities in comparison with the direct problem equations at least for compressible flows. From a numerical viewpoint these features concern the existence of the conservative form of the equations, linearity and specific boundary conditions or sources. From the flow field structure viewpoint, there are also sizable differences, for example, the compression shock formation in adjoint variables field is impossible when the rarefaction shock is stable and exists. The latter effect poses some restrictions on the solution of inverse problems.

Keywords: Adjoint model, discontinuous flow, adjoint model characteristics, Euler equations.

1. Introduction

The discontinuities of gas-dynamic parameters are specific for supersonic flows of inviscid gas. The influence of discontinuities on the gradients of the variables or cost functional is of current interest for both the direct and inverse gas-dynamics problems. For example, Ref. [1] concerns the sensitivity of one-dimensional Euler equations from the viewpoint of the tangent equations. Ref [2] deals with optimal control of shocked flow using smooth and nonsmooth optimization algorithms. Ref. [3] concerns the choice of numerical scheme for the solution of adjoint shallow water equations from viewpoint of gradient of the cost functional.

The present paper concerns the discontinuities of adjoint parameters from viewpoint of the cost functional gradient, which is widely used in the variational statements of inverse problems. These discontinuities may be engendered by discontinuous structures in the gas flow. Another discontinuities may be caused by boundary conditions (sources) in the adjoint problem containing the mismatch between the target and calculated values.

The different forms of adjoint problem that may be obtained from use of either the conservative or non-conservative gas dynamic systems are discussed from the standpoint of discontinuity handling.

2. Model problem statement

We consider the estimation of inlet flow parameters from outflow measurements for supersonic gas flow as the model problem requiring the calculation of the adjoint parameters in an inverse problem. The non-divergent direct problem equations are used at the first step.

$$\rho \frac{\partial U^k}{\partial X^k} + U^k \frac{\partial \rho}{\partial X^k} = 0 \tag{1}$$

$$U^k \frac{\partial U^i}{\partial X^k} + \frac{1}{\rho} \frac{\partial P}{\partial X^i} = 0\,,\ i=1,2 \tag{2}$$

$$U^k \frac{\partial e}{\partial X^k} + (\kappa - 1) e \frac{\partial U^k}{\partial X^k} = 0 \tag{3}$$

$P=\rho RT,\ \ e= C_v T= R/(\kappa-1)T.$

$f(0,Y)= f_\infty (Y);\ f(X,1)= f_\infty (1);\ f(X,0)= f_\infty(0);$ The boundary conditions of the undisturbed external flow are used on boundaries $Y=0,\ Y=1$.

The calculation region sketch is presented in Fig. 1. We are searching to estimate inflow *(X=0)* parameters $\boldsymbol{f}_{\infty}(Y)=(\rho(Y),U_i(Y),e(Y))$ from outflow data $\boldsymbol{f}^{exp}(Y,X_{max}.)$.

The problem is posed as a variational statement of the problem of minimizing the following cost functional:

$$\varepsilon(\boldsymbol{f}_{\infty}(Y)) = \int_{X_{\max}} \left(\boldsymbol{f}(X_{\max}, Y) - \boldsymbol{f}^{\boldsymbol{exp}}(Y)\right)^2 dy \tag{4}$$

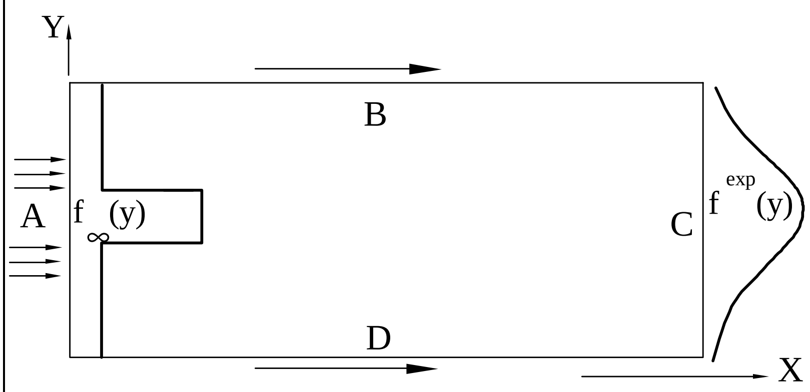

Fig. 1

The gradient of the above cost functional required for its minimization may be obtained from the adjoint equations as described in [4,5].

$$\frac{\partial(\Psi_{\rho}U^k)}{\partial X^k} - \Psi_{\rho}\frac{\partial U^k}{\partial X^k} + (\gamma-1)\left(e\frac{\partial}{\partial X^i}\frac{\Psi_i}{\rho}\right) + \frac{1}{\rho^2}\frac{\partial P}{\partial X^i}\Psi_i = 0 \tag{5}$$

$$\frac{\partial\left(U^k\Psi_i\right)}{\partial X^k} - \frac{\partial U^k}{\partial X^i}\Psi_k + \frac{\partial(\Psi_{\rho}\rho)}{\partial X^i} - \Psi_{\rho}\frac{\partial\rho}{\partial X^i} - \frac{\partial e}{\partial X^i}\Psi_e + (\gamma-1)\frac{\partial\left(\Psi_e e\right)}{\partial X^i} = 0 \tag{6}$$

$$\frac{\partial(U_k\Psi_e)}{\partial X_k}-(\gamma-1)\frac{\partial U_k}{\partial X_k}\Psi_e+(\gamma-1)\rho\frac{\partial}{\partial X_k}\left(\frac{\Psi_k}{\rho}\right)=0 \tag{7}$$

Initial conditions for adjoint problem ($X=X_{max}$) are:

$$\left(U\Psi_\rho+(\gamma-1)\Psi_U e/\rho-2(\rho^{exp}(Y,Z)-\rho(Y,Z))\right)\Big|^{X_{\max}}=0;$$

$$\left(U\Psi_U+\Psi_\rho\rho+\Psi_e(\gamma-1)e-2(U^{exp}(Y,Z)-U(X,Y,Z))\right)\Big|^{X_{\max}}=0;$$

(8)

$$\left(U\Psi_V-2(V^{exp}(Y,Z)-V(Y,Z))\right)\Big|^{X_{\max}}=0;$$

$$\left(U\Psi_e+(\gamma-1)\Psi_U-2\left(e^{exp}(Y,Z)-e(Y,Z)\right)\right)\Big|^{X_{\max}}=0;$$

The boundary *(Y=0; Y=1)* conditions are:

$$\left(\rho\Psi_\rho+\frac{P}{\rho}\Psi_e\right)\Big|_{Y=0}=0;\quad \left(\Psi_V\right)\Big|_{Y=0}=0; \tag{9}$$

The variation of the cost follows:

$$\Delta\varepsilon(\boldsymbol{f}_\infty(Y))=\int_Y\left(\left(\Psi_e U+(\gamma-1)\Psi_U\right)\Delta e_\infty(Y)\right)\Big|_{X=0}dY+$$

$$+\int_Y\left(\left(\Psi_\rho U+(\gamma-1)\Psi_U e/\rho\right)\Delta\rho_\infty(Y)\right)\Big|_{X=0}dY+ \tag{10}$$

$$+\int_Y\left(\left(\Psi_U U+\rho\Psi_\rho+(\gamma-1)\Psi_e e\right)\Delta U_\infty(Y)\right)\Big|_{X=0}dY+\int_Y\left(\Psi_V U\Delta V_\infty(Y)\right)\Big|_{X=0}dY$$

This equation provides the values of the gradient of the cost functional, for example the energy component assumes the form:

$$\nabla \varepsilon_e(e_\infty(Y)) = \left(\Psi_e U + (\gamma-1)\Psi_U\right)_{|X=0} \qquad (11)$$

This gradient provides the key element of the inverse problem solution via optimization methods.

System (5-7) has a quasi-conservative form in terms of the adjoint variables. It also has sources, containing spatial derivatives of the gas-dynamic parameters. The discontinuities (both in gas-dynamics system and its adjoint variables) are the cause of computational difficulties when this system is to be solved. The standard ways to handle these difficulties are based on using the divergent equation form or introducing certain viscosity (natural or artificial) [6]. Eqs. (1-3) may be solved by smoothing the gas-dynamic field. If the field is not smooth numerical problems are expected in (5-7) due to the discontinuous coefficients and infinite spatial gradients of the field parameters.

3. Discontinuities of the adjoint parameters

The propagation of the small disturbances in the flow-field is described by characteristics of the tangent linear model [7]. Let us consider the model linear system

$$\iint \left(A_{ij}\frac{\partial U_j}{\partial X} + a_{ij}\frac{\partial U_j}{\partial Y}\right)\Psi_i\,dXdY = -\iint \left(A_{ij}\frac{\partial \Psi_i}{\partial X} + a_{ij}\frac{\partial \Psi_i}{\partial Y}\right)U_j\,dXdY +$$

$$+\int_{\Gamma_1} A_{ij}\Psi_i U_j\,dY + \int_{\Gamma_2} a_{ij}\Psi_i U_j\,dX$$

$$\text{direct problem: } A_{ij}\frac{\partial U_j}{\partial X} + a_{ij}\frac{\partial U_j}{\partial Y} = 0; \qquad (12)$$

$$\text{adjoint problem: } A_{ij}\frac{\partial \Psi_i}{\partial X} + a_{ij}\frac{\partial \Psi_i}{\partial Y} = 0$$

The adjoint problem operators are formed by transposition of the direct problem operators. The characteristics may be determined by the analysis of the propagation of a disturbance of the form $l_i e^{i(\omega x - ky)}$. The characteristic directions are determined by the equation $\left|\lambda A_{ij} - a_{ij}\right| = 0$; $\lambda = \frac{\omega}{k}$ **[**7**].** Thus, the characteristics of the direct and adjoint systems coincide while the adjoint variables evolve along the direct problem characteristics but in the opposite direction. This feature engenders most of the adjoint field peculiarities.

Let us compare the gas-dynamics and its adjoint variables discontinuities formation for the simplest transport equation

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} = 0\,;\; \frac{\partial \Psi}{\partial t} + U\frac{\partial \Psi}{\partial x} = 0 \qquad (13)$$

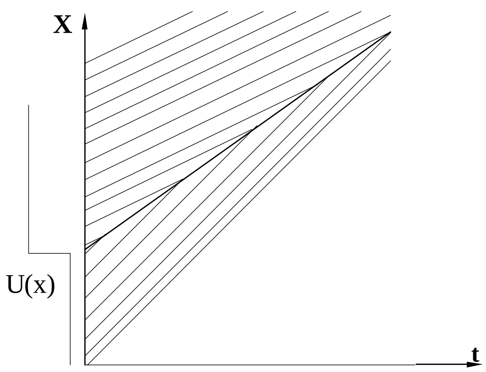

Fig. 2

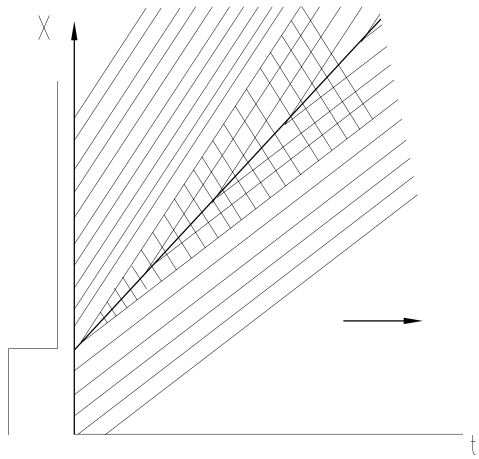

Fig. 3

Figs. 2 presents the shock wave formation for first equation (13). Formally, the rarefaction (expansion) wave (Fig. 3) is its antipode. But the expansion wave is unstable and a small variation of the initial shape *U (x)* transforms it into an expansion (rarefaction) fan (Fig. 4). So, only structures of Fig. 2 and Fig. 4 really appear in gas dynamics.

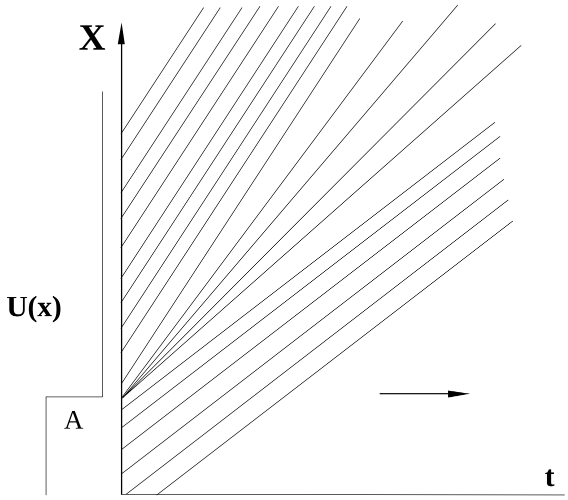

Fig. 4

As the characteristics of adjoint problems are the same as of the direct one, although the evolution occurs in the opposite direction, we have the same characteristic structures in adjoint variables field (Fig. 2, 4). With the account of reverse evolution, a gas-dynamics rarefaction fan corresponds to a compression fan in the adjoint field. Thus, the adjoint parameters may have discontinuity in the single boundary point (point A, Fig. 4). This discontinuity formation and transfer along the other family characteristics were described in [8] for 2-D flow.

On the other hand, the adjoint variables' field should have a rarefaction shock structure (Fig. 3) on the gas-dynamics shock due to reverse evolution. In this case, the shock is stable since the coefficients in adjoint equations are derived from the previously computed gas-dynamics field. A single value of adjoint parameter determines in this way a total segment in the adjoint field (Fig. 3). So, the adjoint variables (and the cost functional gradient) are degenerate in this segment, a fact that may cause numerical difficulties in the optimization process although the adjoint parameters are continuous on this structure. For example, if we look for an initial distribution $U(x)$ from certain final observation $U^{\exp}(T,x)$ the gradient of the cost functional may be expressed as $\nabla\varepsilon(U(x)) = -\Psi(0,x)$. The abovementioned degeneration causes a constant value of gradient in significant vicinity of the discontinuity causing the impossibility of exact restoration of the initial profile $U\ (x)$.

For the two dimensional supersonic flow (Fig. 1, equations (1-3)), the direct and the adjoint field structures are presented in Figs. 5 and 6. Fig. 5 describes the rarefaction fan in gas-dynamics parameters and the compression fan in the adjoint field (the discontinuity from boundary point A is transferred into the flow-field along the characteristic C_+. Fig. 6 describes the shock wave in the gas-dynamics variables and the expansion (rarefaction) shock in the adjoint variables field.

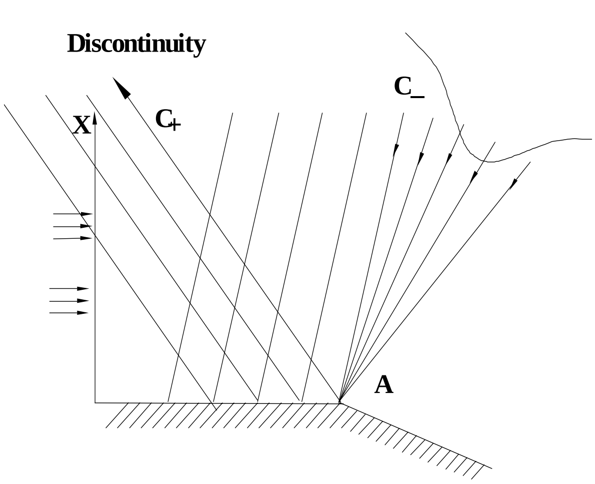

Fig. 5

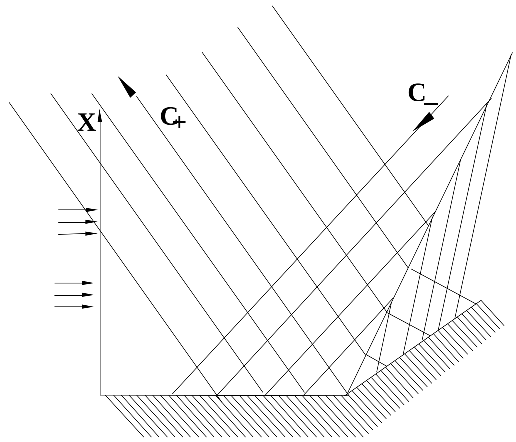

Fig. 6

The adjoint equations in inverse problems are loaded by the mismatch between target and calculated values, which may occur in the boundary conditions (Eqs. 8) or in source terms in the flow field. Both target and calculated values may have discontinuities. Naturally, these discontinuities propagate along characteristics.

4. Numerical Tests

The formation of the shock waves (even from an initially gently sloping shape) is the feature of the considered equations. This process should cause the loss of information regarding initial parameter distribution when the inverse problem is solved. In the adjoint problem this appears in the solution, which is degenerate in the hatched sector (Fig. 3). So, when the inverse problem is solved, numerical difficulties (instability or lack of convergence, for example) appear. The information losses in such structure should increase as the shock intensity increases. This aspect was verified by carrying out some numerical tests.

For the flow-field calculation we used a nondivergent finite-difference approximation of the parabolized Navier-Stokes equations [3,4]. The main deviation from the system (1-3) consists in the viscous terms $\frac{1}{\mathrm{Re}\,\rho}\frac{\partial^2 U^i}{\partial X_k^2}\delta_{2k}$ (Re=10^4) used to smooth the shocks.

Fig. 7 presents the isolines of the adjoint density caused by the jump in the target parameters on the outflow boundary. Both the contact line discontinuities and discontinuities moving along the sound characteristics are visible.

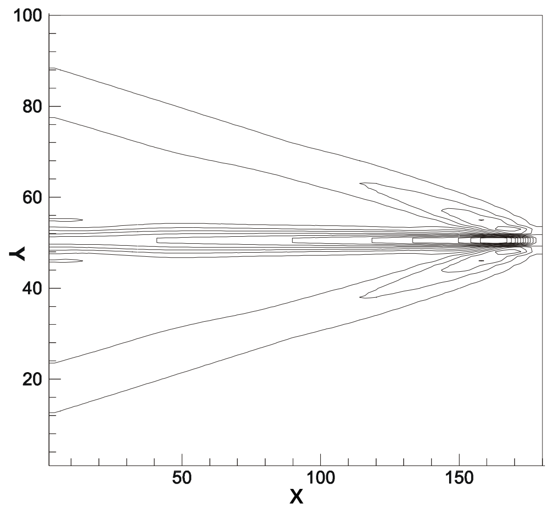

Fig. 7

Fig. 8 provides the density isolines for the expansion fan. Fig. 9 demonstrates the corresponding adjoint density field. The high gradients zone (smeared adjoint density discontinuity) appears in the expansion fan focus and spreads further along the characteristics.

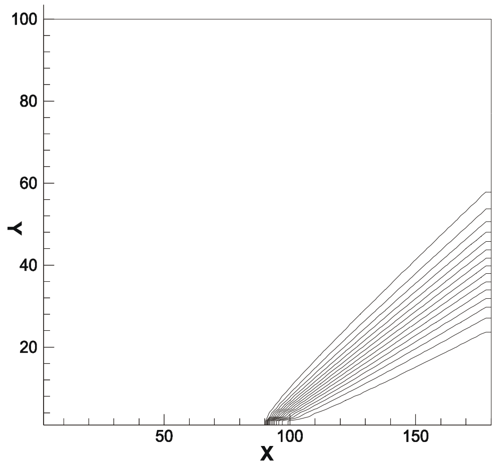

Fig. 8

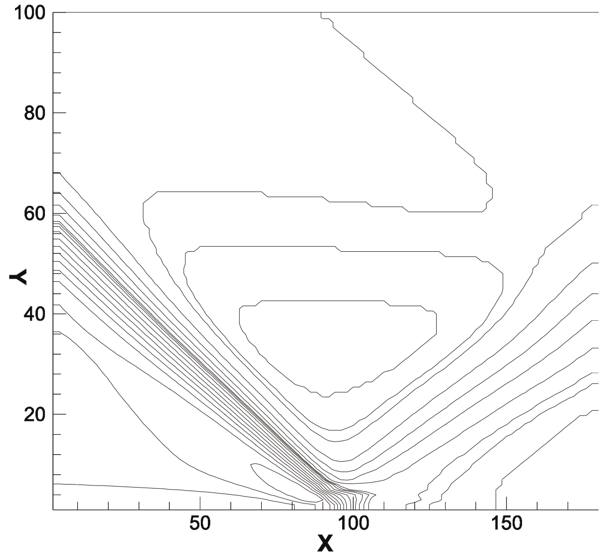

Fig. 9

As previously mentioned, the shock formation causes an irreversible loss of information regarding the initial parameters. The impact of the shock on the quality of the inverse problem solution is estimated from this viewpoint. The gradient was obtained from the adjoint field while the optimization was performed using the L-BGGS limited-memory quasi-Newton method [9].

Numerical tests demonstrate that the quality of the solution deteriorates as the shock intensity increases. This process is similar to information losses in viscous processes. A comparison of inverse problem solution quality dependence on nonlinearity (shock intensity), Fig. 10, and viscosity (Reynolds number), Fig. 11, may be investigated. Fig. 10 presents the quality of inflow temperature profile restoration dependence on the ratio of jet temperature (pressure) to the ambient temperature (pressure) in an under-expanded jet (inviscid flow) on the shock intensity. Fig. 11 presents the quality of inflow temperature profile restoration depending on the Reynolds number. We can see that increasing the shock intensity is analogous to increasing the viscosity (i.e. decreasing of Reynolds number).

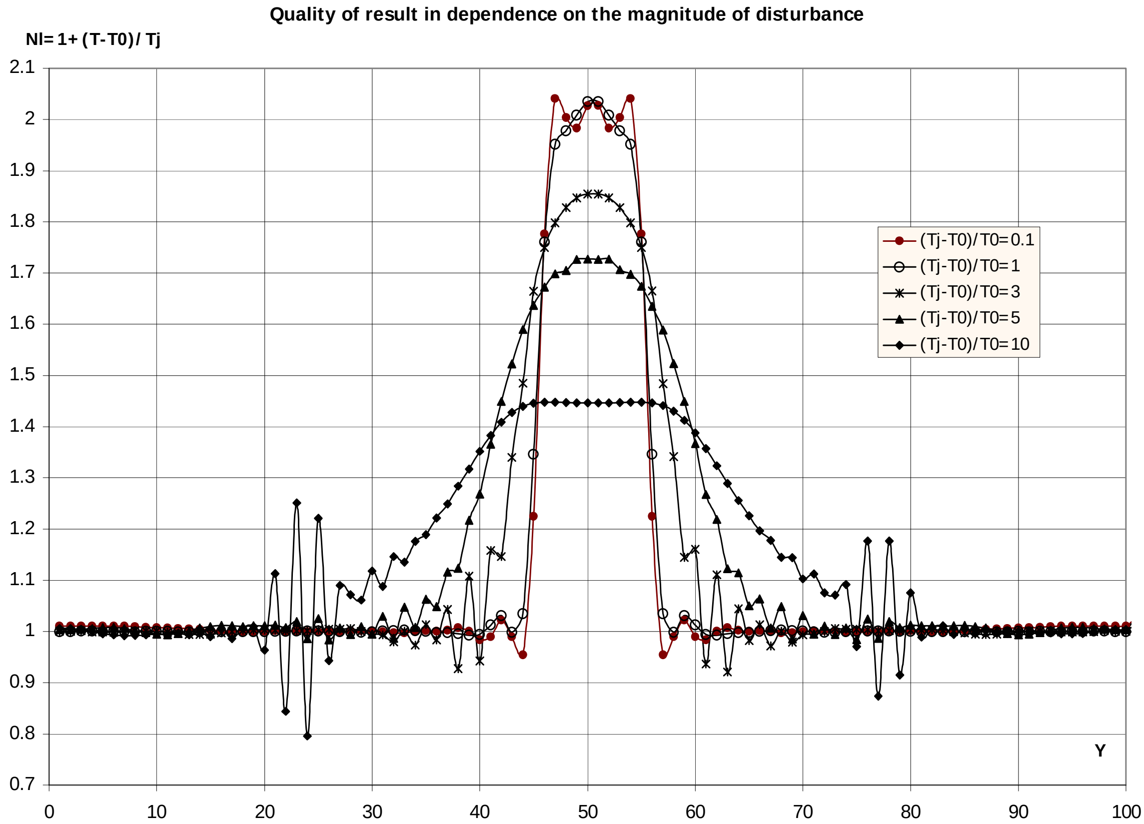
Quality of result in dependence on the magnitude of disturbance
Nl=1+(T-T0)/Tj
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0
10
20
30
40
50
60
70
80
90
100
Y
(Tj-T0)/T0=0.1
(Tj-T0)/T0=1
(Tj-T0)/T0=3
(Tj-T0)/T0=5
(Tj-T0)/T0=10

Fig. 10

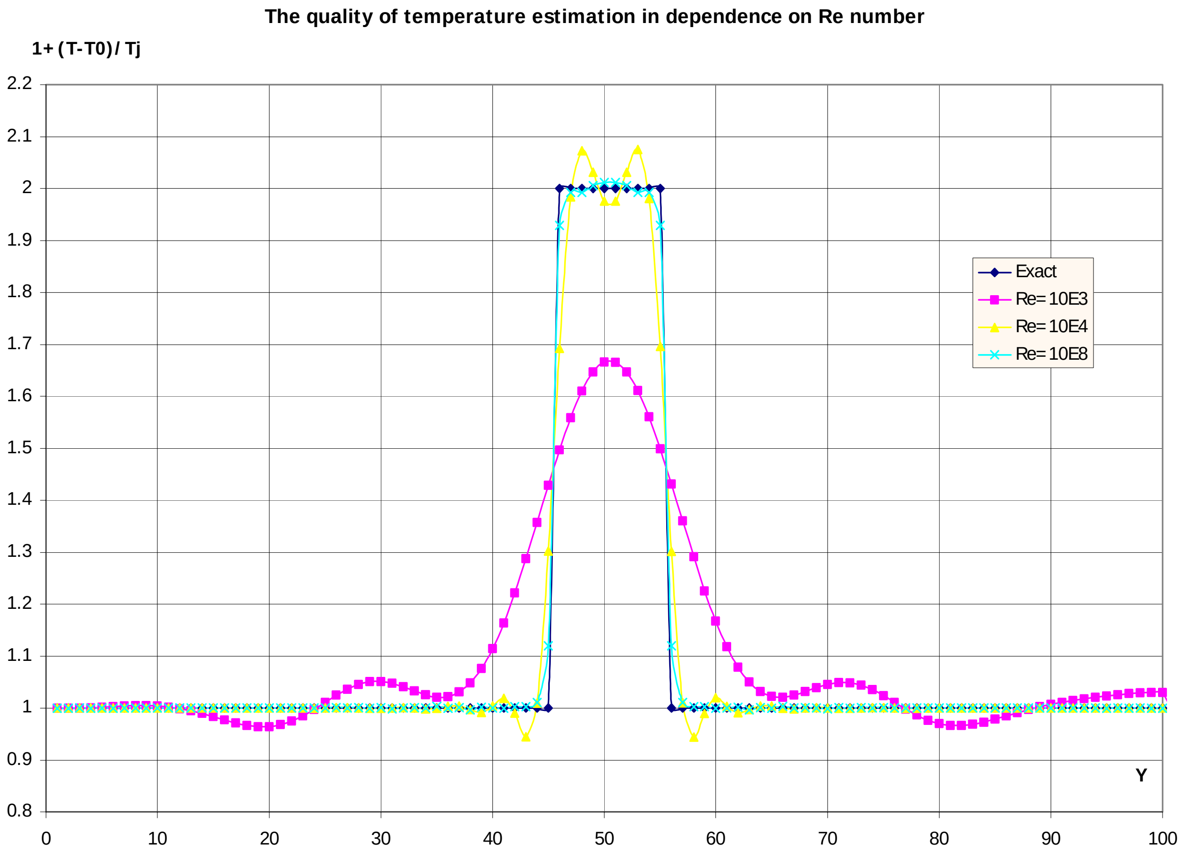

Fig. 11

5. Adjoint problem corresponding to the divergent form of the direct problem

Depending on the form of the direct problem (divergent or non-divergent) the form of the adjoint problem changes. For the non-divergent direct problem

$$A_{ij}(U)\frac{\partial U_j}{\partial X} + a_{ij}(U)\frac{\partial U_j}{\partial Y} = 0 \tag{14}$$

the adjoint problem has a quasi-conservative ([7]) form

$$+\frac{\partial(A_{ij}(U)\Psi_i)}{\partial X} + \frac{\partial(a_{ij}(U)\Psi_i)}{\partial Y} - F_{ij}\Psi_i = 0 \tag{15}$$

where the source terms $F_{ik} = \left(\frac{\partial A_{ij}(U)}{\partial U_k} \frac{\partial U_j}{\partial X} + \frac{\partial a_{ij}(U)}{\partial U_k} \frac{\partial U_j}{\partial Y} \right)$ in general contain the space derivatives of the gas-dynamic parameters. If the direct problem is smeared (i.e. has no discontinuities) the adjoint equations do not contain any singularities.

For the direct problem conservative form,

$$\frac{\partial (B_{ij}(U)U_j)}{\partial X} + \frac{\partial (B_{ij}(U)U_j)}{\partial Y} = 0 \qquad (16)$$

the adjoint problem has a nondivergent form containing no space derivatives of the gas-dynamic parameters.

$$(B_{ij}(U) + G_{ij}) \frac{\partial \Psi_i}{\partial X} + (b_{ij}(U) + M_{ij}) \frac{\partial \Psi_i}{\partial Y} = 0 \qquad (17)$$

where $G_{ik} = \frac{\partial B_{ij}(U)}{\partial U_k} U_j$; $M_{ik} = \frac{\partial b_{ij}(U)}{\partial U_k} U_j$.

The adjoint variables should be smeared for the shock-capturing calculations.

Thus, in inverse problems the shock-capturing means smoothing either the direct problem variables or the adjoint variables. From this viewpoint, the use of automatic differentiation for compressible inviscid flows requires the exercise of some caution. We may have no difficulties with discontinuities in the divergent direct problem but the corresponding adjoint problem should use additional means to handle discontinuities.

It should be mentioned that when the adjoint problem is obtained from the divergent direct one, the sources (at the boundary or within the flow field) are engendered only by the discrepancy between calculation and target a fact that may be turn to be very useful during debugging.

Ref. [3] discusses the choice of numerical schemes for the solution of adjoint shallow water equations. The adjoint equations corresponding to the conservative form of direct equations are not conservative. The special finite volume method was successfully used for approximation of the adjoint equations. Ref [11] deals with optimal boundary control of aeroacoustic noise governed by the two-dimensional unsteady compressible Euler equations. We have above considered the couple of non-divergent direct problem (1-3) and quasi-conservative adjoint problem (5-7) for gas flow. Let us now compare the couple of divergent direct problem (18-20) and non-divergent adjoint one (23-25). The system (18-20) provides for the calculation of discontinuities without smearing.

$$\frac{\partial\left(\rho U^k\right)}{\partial X^k}=0 \tag{18}$$

$$\frac{\partial\left(\rho U^k U^i+P\delta_{ik}\right)}{\partial X^k}=0 \tag{19}$$

$$\frac{\partial\left(\rho U^k h_0\right)}{\partial X^k}=0\,; \tag{20}$$

Here $h(\rho,P)=\frac{\gamma}{\gamma-1}\frac{P}{\rho}$ is gas specific enthalpy, $h_0=h+(U^2+V^2)/2$ - total enthalpy, $P=\rho RT$, $P=\rho(\gamma-1)/\gamma(h_0-(U^2+V^2)/2)$, $e=R/(\gamma-1)T$, $h=\gamma e$.

In a standard way, we form Lagrangian $L(\mathbf{f}_\infty(Y))$ from the cost functional and the weak statement of (18-20).

$$L\left(f_\infty(Y)\right)=\varepsilon(f_\infty(Y))+\int_\Omega\left(\frac{\partial\left(\rho U^k\right)}{\partial X^k}\right)\Psi_\rho\, d\Omega$$
$$+\int_\Omega\left(\frac{\partial\left(\rho U^k U^i+P\delta_{ik}\right)}{\partial X^k}\right)\Psi_i d\Omega+\int_\Omega\frac{\partial\left(\rho U^k h_0\right)}{\partial X^k}\Psi_h d\Omega \tag{21}$$

The Lagrangian is transformed by the integration by parts

$$L\left(f_\infty(Y)\right)=\varepsilon(f_\infty(Y))-\int_\Omega\left(\frac{\partial\Psi_\rho}{\partial X^k}\right)\rho U^k\, d\Omega+\int_{\sigma_k}\Psi_\rho\rho U^k\Big|_{X_k=0}^{X_k^{\max}} d\sigma_k$$

$$-\int_{\Omega}\left(\frac{\partial\Psi_i}{\partial X^k}(\rho U^k U^i + P\delta_{ik})\right)d\Omega + \int_{\sigma_k}\Psi_i(\rho U^k U^i + P\delta_{ik})\Big|_{X_k=0}^{X_k^{\max}} d\sigma_k$$

$$-\int_{\Omega}\frac{\partial\Psi_h}{\partial X^k}\left(\rho U^k h_0\right)d\Omega + \int_{\sigma_k}\Psi_h \rho U^k h_0\Big|_{X_k=0}^{X_k^{\max}} d\sigma_k \tag{22}$$

This form is very useful for finding the variation of the Lagrangian for a comparison starting from the nondivergent flow equations. The adjoint parameters $(\Psi_\rho, \Psi_U, \Psi_V, \Psi_h)$ provide conditions for Lagrangian variation to depend on control parameters in the form $\Delta L=\Delta\varepsilon=\int_{Y,Z} grad(\varepsilon)\Delta f_\infty(Y)dY$. The adjoint variables should satisfy the following system

$$U^k\frac{\partial\Psi_\rho}{\partial X^k} + U^k U^i\frac{\partial\Psi_i}{\partial X^k} + \frac{\gamma-1}{\gamma}\frac{\partial\Psi_k}{\partial X^k}\left(h_0 - U_n U_n/2\right) + U^k h_0\frac{\partial\Psi_h}{\partial X^k} = 0 \tag{23}$$

$$\rho U^i\frac{\partial\Psi_i}{\partial X^k} + \rho U^i\frac{\partial\Psi_k}{\partial X^i} + \rho\frac{\partial\Psi_\rho}{\partial X^k} + \frac{\gamma-1}{\gamma}\frac{\partial\Psi_i}{\partial X^n}\delta_{in}\rho U_k + \rho h_0\frac{\partial\Psi_h}{\partial X^k} = 0 \tag{24}$$

$$\rho U^k\frac{\partial\Psi_h}{\partial X^k} + \frac{\gamma-1}{\gamma}\rho\frac{\partial\Psi_k}{\partial X^k} = 0 \tag{25}$$

Initial conditions for the adjoint problem are posed on outflow boundary ($X=X_{max}$).

$$(\Psi_\rho U^x + \Psi_i U^x U^i + \frac{\gamma-1}{\gamma}\Psi_x\left(h_0 - U_n U_n/2\right) + \Psi_h U^x h_0 - 2(\rho(Y) - \rho^{exp}(Y)))\Big|^{X_{\max}} = 0;$$

$$\left(\rho\Psi_\rho\delta_{ix} + \rho\Psi_n U^n\delta_{ix} + \rho\Psi_i U^x - \frac{\gamma-1}{\gamma}\rho\Psi_x U_i + \Psi_h\rho h_0\delta_{ix} - 2(U^i(Y) - U^i_{\exp}(Y))\right)^{X_{\max}} = 0;\ i=1,2 \tag{26}$$

$$\left(\frac{\gamma-1}{\gamma}\Psi_x\rho + \Psi_h\rho U^x - 2\left(h_0(Y) - h_0^{exp}(Y)\right)\right)\Big|^{X_{\max}} = 0;$$

The boundary conditions at *(Y=0;1)* are:

$$\left(\Psi_\rho + \Psi_n U^n + h_0 \Psi_h\right)\Big|_{Y=0} = 0; \quad \left(\Psi_V\right)\Big|_{Y=0} = 0; \tag{27}$$

The cost functional variation is :

$$\Delta\varepsilon(\boldsymbol{f}_\infty(Y,Z)) = \int_\Omega \left(\left(\Psi_\rho U^x + \Psi_i U^x U^i + \frac{\gamma-1}{\gamma}\Psi_x\left(h_0 - U_n U_n/2\right) + \Psi_h U^x h_0\right)\Delta\rho_\infty(Y)\right)\Big|_{X=0} dY +$$

$$+\int_\Omega \left(\left(\rho\Psi_\rho\delta_{ix} + \rho\Psi_n U^n\delta_{ix} + \rho\Psi_i U^x - \frac{\gamma-1}{\gamma}\rho\Psi_x U_i + \Psi_h\rho h_0\delta_{ix} - 2(U^i(Y) - U^i_{\exp}(Y))\right)\Delta U^i{}_\infty(Y)\right)\Big|_{X=0} dY +$$

$$+\int_\Omega \left(\left(\frac{\gamma-1}{\gamma}\Psi_x\rho + \Psi_h\rho U^x\right)\Delta h^0{}_\infty(Y)\right)\Big|_{X=0} dY \tag{28}$$

The present expression yields the gradient of the cost functional.

The divergent form of direct problem provides for feasibility of shock-capturing calculation. Similarly, the adjoint problem obtained from the divergent form avoids difficulties connected with unbounded spatial derivatives of gas-dynamic parameters that arise in non-divergent form [4,5]. Nevertheless, the adjoint parameters may have their own discontinuities and system (23-25) cannot be computed without additional smoothing or using special numerical schemes [3]. In [3] the smoothing is performed on the direct problem solving for the strong shock and is mentioned there as the reason for convergence rate deterioration. It may be that the real reason for the poorer convergence was the loss of the information in the shock as described above.

The comparison of direct and adjoint forms of equations is presented in the Table 1.

Table 1

Direct problem (D1)	Adjoint problem (A1)
$\rho \frac{\partial U^k}{\partial X^k} + U^k \frac{\partial \rho}{\partial X^k} = 0$	$\frac{\partial(\Psi_\rho U^k)}{\partial X^k} - \Psi_\rho \frac{\partial U^k}{\partial X^k} + (\gamma-1)\left(e\frac{\partial}{\partial X^k}\frac{\Psi_k}{\rho}\right) + \frac{1}{\rho^2}\frac{\partial(\rho e(\gamma-1))}{\partial X^k}\Psi_k = 0$
$U^k \frac{\partial U^i}{\partial X^k} + \frac{(\gamma-1)}{\rho}\frac{\partial(\rho e)}{\partial X^i} = 0$	$\frac{\partial\left(U^k\Psi_i\right)}{\partial X^k} - \frac{\partial U^k}{\partial X^i}\Psi_k + \frac{\partial(\Psi_\rho \rho)}{\partial X^i} - \Psi_\rho\frac{\partial\rho}{\partial X^i} - \frac{\partial e}{\partial X^i}\Psi_e + (\gamma-1)\frac{\partial\left(\Psi_e e\right)}{\partial X^i} = 0$
$U^k\frac{\partial e}{\partial X^k} + (\gamma-1)e\frac{\partial U^k}{\partial X^k} = 0$	$\frac{\partial(U_k\Psi_e)}{\partial X_k} - (\gamma-1)\frac{\partial U_k}{\partial X_k}\Psi_e + (\gamma-1)\rho\frac{\partial}{\partial X_k}\left(\frac{\Psi_k}{\rho}\right) = 0$
Spatial derivatives of discontinuous field parameters $\frac{\partial\rho}{\partial X^i}$ are available. Discontinuous coefficients in expressions $\frac{\partial\left(U^k\Psi_i\right)}{\partial X^k}$ are compensated by discontinuities in adjoint parameters and the spatial derivatives do not engender the singularities.	

Direct problem (D2)	Adjoint problem (A2)
$\frac{\partial\left(\rho U^k\right)}{\partial X^k} = 0$	$U^k\frac{\partial\Psi_\rho}{\partial X^k} + U^k U^i\frac{\partial\Psi_i}{\partial X^k} + \frac{\gamma-1}{\gamma}\frac{\partial\Psi_k}{\partial X^k}\left(h_0 - U_n U_n/2\right) + U^k h_0\frac{\partial\Psi_h}{\partial X^k} = 0$
$\frac{\partial\left(\rho U^k U^i + P\delta_{ik}\right)}{\partial X^k} = 0$	$U^i\frac{\partial\Psi_i}{\partial X^k} + U^i\frac{\partial\Psi_k}{\partial X^i} + \frac{\partial\Psi_\rho}{\partial X^k} + \frac{\gamma-1}{\gamma}\frac{\partial\Psi_i}{\partial X^n}\delta_{in}U_k + h_0\frac{\partial\Psi_h}{\partial X^k} = 0$
$\frac{\partial\left(\rho U^k h_0\right)}{\partial X^k} = 0$;	$U^k\frac{\partial\Psi_h}{\partial X^k} + \frac{\gamma-1}{\gamma}\frac{\partial\Psi_k}{\partial X^k} = 0$
Spatial derivatives of discontinuous adjoint parameters $\frac{\partial\Psi_i}{\partial X^k}$ are present.	

At first glance the direct and adjoint problems appear to be inseparably linked. Nevertheless, if we have fixed (codes, for example) adjoint system (A1 or A2) we may use any (most suitable) direct problem since the gas-dynamics parameters (from D1 and D2) are easily converted. Conversion of adjoint parameters is barely feasible, hence if the direct problem is fixed, there is no choice in adjoint problem.

CONCLUSION

The computation of the adjoint variables for supersonic inviscid equations is complicated by the existence of discontinuities both in the gas-dynamic field and in the adjoint field. The discontinuities of the adjoint variables are of the following kinds:

1. Discontinuities moving along streamline and discontinuities, moving along sonic lines from the breaks of the target functions (on boundary or within flow-field).
2. A discontinuity, arising on the boundary at the focus of the expansion fan and transferred within the flow field along the characteristics of another family.

These discontinuities pose significant numerical difficulties for the calculation of the adjoint field parameters. Different forms of the adjoint problem exist, which are not equivalent from the numerical viewpoint:

1. Direct problem divergent form (Eqs. 21-23) engenders non-divergent adjoint equations, which should have computational problem with the discontinuities of adjoint parameters. On the other hand, this form does not contain space derivatives of gasdynamic parameters and is thus tolerant to flow discontinuity. Special numerical schemes are efficient for this form of equations [3].

2. The non-divergent form of the direct problem yields quasi-conservative form of the adjoint problem, which has no problem with the adjoint parameter discontinuity, but is having sources containing gas-dynamic parameters' spatial derivatives, which are unbounded on the discontinuities.

In both events special means to handle the discontinuities must be used. Special attention should be paid to the implementation of automatic differentiation tools for the compressible flows described by the divergent equations. In this event, the corresponding adjoint problem is not divergent and has numerical difficulties related to the adjoint parameters' discontinuities.

The shock formation causes an irreversible loss of information. This phenomenon is similar to the information loss in the dissipation. For the adjoint problem calculation this effect arises as the degeneration of the adjoint parameters within an expansion wave and causes the deterioration of the quality of inverse problem solution.

Use of nonsmooth optimization algorithm as in [2] or in [10] can serve as a useful tool to handle discontinuities and to avoid use of smoothing.

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