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Difficulties in Sensitivity Calculations for Flows with Discontinuities

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The use of flow sensitivities has become an integral part of flow optimization-based aerodynamic design and is useful for the efficient calculation of perturbed flows. However, there are still many issues to be resolved, especially for flows having discontinuities. Flow sensitivities for several numerical methods are calculated using finite difference quotients, automatic differentiation, and the sensitivity equation method. The flow sensitivities are calculated for the Riemann problem of gas dynamics. An attempt is made to expose, explain, and understand difficulties that arise in the calculation of flow sensitivities in flows with discontinuities.

Nomenclature

$A(U)$	= flux Jacobian
$\bar{A}(U_i, U_{i+1})$	= Roe-averaged Jacobian for Roe scheme
e	= energy per unit volume
e'	= energy per unit volume sensitivity
e_j	= energy per unit volume in region j
e'_j	= energy per unit volume sensitivity in region j, $\partial e_j/\partial P_4$
$F(U)$	= flux vector
F_i^*	= discrete Roe flux vector
$F_i^n(U_i^n)$	= discrete flux vector
$G(U, S)$	= sensitivity flux vector, $(\partial F/\partial P_4)(U)$
$G_i^n(U_i^n, S_i^n)$	= discrete sensitivity flux vector, $(\partial F_i^n/\partial P_4)(U_i^n)$
m	= momentum
m'	= momentum sensitivity
m_j	= momentum in region j
m'_j	= momentum sensitivity in region j, $\partial m_j/\partial P_4$
P	= pressure
P'	= pressure sensitivity
P_j	= pressure in region j
P'_j	= pressure sensitivity in region j, $\partial P_j/\partial P_4$
$\bar{r}_j$	= eigenvectors of $\bar{A}$
S	= flow sensitivity vector, $\partial U/\partial \alpha$
S_i^n	= discrete sensitivity vector, $\partial U_i^n/\partial \alpha$
t	= temporal variable
U	= conservative flow vector
U_i^n	= discrete conservative flow vector
$(U_\alpha)^h$	= differentiate-then-discretize sensitivity
$(U^h)_\alpha$	= discretize-then-differentiate sensitivity
u	= velocity
u'	= velocity sensitivity
u_j	= velocity in region j
u'_j	= velocity sensitivity in region j, $\partial u_j/\partial P_4$
x	= spatial variable
$x_s(\alpha)$	= shock location
α	= sensitivity parameter
γ	= ratio of specific heats
ϵ	= internal energy per unit mass
$\bar{\lambda}_j$	= eigenvalues of $\bar{A}$
ν	= Lapidus artificial viscosity constant
ρ	= density
ρ'	= density sensitivity
ρ_j	= density in region j
ρ'_j	= density sensitivity in region j, $\partial \rho_j/\partial P_4$

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I. Introduction

FLOW sensitivities, i.e., the derivatives of the variables that describe the flow with respect to parameters that determine the flow, are useful in at least three settings. First, they are interesting in their own right because they tell the engineer what, when, and where these parameters most influence the flow. Second, they can be used in a Taylor series or some other similar setting to determine nearby flows; i.e., given the flow variables and their sensitivities at specified values of the parameters, one can determine approximations to the flow variables at nearby values of the parameters. Certain methods for computing the sensitivities result in the determination of the nearby flow at much less cost compared with doing a full-fledged flow solution at the new value of the parameters. Taylor et al.[1] and Burgreen[2] considered this problem using a linear approximant for the nearby flow in the prescence of discontinuities and gave examples of how the discontinuity affects different problems. Third, flow sensitivities can be used within an optimization or control setting to help determine the gradient of the objective functional with respect to the parameters that participate in the optimization process. This is an evergrowing area that has recently received much attention.[3] Some of the major contributors include Bischof et al.,[4] Newman and Taylor,[5,6] Eyi and Lee,[7] Borggaard,[8] Borggaard et al.,[9] Burkardt,[10] and Appel et al.[11] Narducci et al.[12] have considered designs in which the shock must be taken into account.

In each of the aforementioned applications, difficulties arise in the calculation and use of sensitivities for flows with discontinuities. Clearly, the importance and usefulness of flow sensitivities in optimization-based design have been demonstrated. Furthermore, it seems that the gross inaccuracies in sensitivity approximations that result directly from approximate flow discontinuities do not prevent the convergence of gradient-based optimization schemes. However, for sensitivities to be a truly useful tool in the other two contexts, there will need to be improvements made on how sensitivities are defined, computed, and utilized. In fact, if one applies currently available sensitivity approximation methodologies to flows containing discontinuities, one cannot obtain meaningful approximations to nearby flows or accurate enough sensitivities to be of use in the first context discussed earlier. Thus, although improvements in sensitivity approximations will also result in better performance of optimization processes, this paper is devoted to the understanding of flow sensitivities and their approximation in general and not only to optimization-based design.

The first step in improving and correcting algorithms for determining and using approximate sensitivities is gaining an understanding of how they are affected by different flow phenomena and calculation methods. This is the subject of this paper.

II. Sensitivity Methodologies

Computational calculation methods for determining approximate flow sensitivities can be divided into two classes. The first is the discretize-then-differentiate approach. In this class of methods, the discrete equations for the approximate flow solution $\boldsymbol{U}^h$ are differentiated with respect to a parameter α to determine a discrete set of equations for the approximate sensitivity $(\boldsymbol{U}^h)_\alpha$. There are three prominent methods in this class. The first is based on hand-differentiating the discrete flow equations to produce a set of discrete equations for the approximate flow sensitivity. Because hand-differentiation is often difficult, e.g., due to complications ensuing from turbulence models or numerical shock capturing treatments, a second method is based on automatic differentiation methodologies, e.g., ADIFOR,[4] which, in effect, apply the chain rule to differentiate the flow simulation code with respect to a parameter α to produce a new code that not only determines approximate flow solutions but also the exact (to roundoff error) discrete sensitivity $(\boldsymbol{U}^h)_\alpha$. The third method in this class is the finite difference quotient approach wherein approximate sensitivities are calculated by perturbing the original parameter value α by an amount $\Delta\alpha$ and then applying a standard finite different quotient formula, e.g., $(\boldsymbol{U}^h)_\alpha \approx [\boldsymbol{U}^h(\alpha+\Delta\alpha) - \boldsymbol{U}^h(\alpha)]/\Delta\alpha$. The belief is that as $\Delta\alpha \to 0$, the finite difference sensitivity will approach the exact discrete sensitivity $(\boldsymbol{U}^h)_\alpha$.

The second class of sensitivity calculation methods is the differentiate-then-discretize approach. In this class of methods, the governing system of (continuous) partial differential equations modeling the flow $\boldsymbol{U}$ are differentiated with respect to a parameter α to obtain a system, which we refer to as the continuous sensitivity equations, of linear partial differential equations for the exact flow sensitivity $\boldsymbol{U}_\alpha$. This system can then be discretized, either by a method similar to that used for the flow simulation or by a different method, to obtain an approximate sensitivity $(\boldsymbol{U}_\alpha)^h$. This type of approach is referred to as the sensitivity equations method.

Note that, in general, $(\boldsymbol{U}^h)_\alpha \neq (\boldsymbol{U}_\alpha)^h$, a fact that may lead to difficulties.[8,10,13] Also note that all of the approaches discussed earlier only produce approximations to the true sensitivities of the continuous flow $\boldsymbol{U}_\alpha$. On the other hand, an approach such as the automatic differentiation (but not finite difference quotients) will produce, to roundoff error, the exact sensitivities $(\boldsymbol{U}^h)_\alpha$ of the discrete flow $\boldsymbol{U}^h$, whereas the differentiate-then-discretize approach will not produce any kind of exact sensitivity.

In different settings, one or another type of approximate sensitivity methodology may be preferable. For example, within the optimization setting, one may be required to supply the gradient of a discretized functional. In this case, the use of a gradient computed with the aid of sensitivities obtained through a discretize-then-differentiate approach (e.g., automatic differentiation) can be, to roundoff error, the exact gradient of the discrete functional. On the other hand, functional gradients obtained with the help of sensitivities that are calculated through the differentiate-then-discretize approach will not, in general, be exact gradients of either the continuous or discretized functionals. This inconsistency can, on occasion, cause difficulties with an optimization process. However, this potential difficulty should be weighed against the facts that the sensitivity equation approach will yield sensitivities at a much lower cost than through the use of finite difference quotients and that the cost of using an automatic differentiation approach can sometimes be comparable to the latter. In an optimization problem for which the objective functional is highly discontinuous or oscillatory, it is often preferable to use a nongradient-based optimization technique such as a direct search method.[14] The emphasis here should be on the bad behavior of the objective functional for which the notion of a gradient is somewhat meaningless[15] as opposed to inviscid, compressible flow optimizations involving discontinuous flows for which the gradient is meaningful almost everywhere.[11] Direct methods are usually very robust but converge at a much slower rate and are too costly to solve optimization problems with a large number of parameters or with very costly state, i.e., flow, solves. In any case, both the sensitivity equation approach,[8,9,11] despite the potential for gradient inconsistencies, and the automatic differentiation approach,[4] despite its greater cost, have been shown to be viable and robust methods of providing sensitivities for useful and effective gradient-based flow optimization algorithms, including inviscid, compressible flows with discontinuities.

Another issue that arises in discretize-then-differentiate vs differentiate-then-discretize comparisons is the issue of the differentiation of terms added to the flow equations for the sake of computational expediency. We refer to these as computational facilitators, examples of which are turbulence models and shock capturing mechanisms such as flux limiters. Note that these are usually highly complex and nonlinear. When using the discretize-then-differentiate approach, it is difficult to avoid differentiating computational facilitators, and, indeed, attempts at avoiding them can negate some of the simplicity of using automatic differentiation. On the other hand, with the sensitivity equation method one can easily ignore computational facilitators and differentiate the basic governing equations, e.g., Euler or Navier–Stokes. (One may, if needed, then introduce nondifferentiated computational facilitators into the sensitivity equations.) In this paper we point out inaccuracies in computed sensitivities that result from flow discontinuities. Related to the computational facilitator issue is the implementation of methods for overcoming these inaccuracies; this again is difficult to do in the automatic differentiation setting without negating some of its advantages and may be easier to do within sensitivity equation methods.

If one really wants to know the sensitivities themselves, one would, of course, prefer to have in hand the true flow sensitivities $\boldsymbol{U}_\alpha$ just the same as one would like to know the true flow $\boldsymbol{U}$. Because these are usually impossible to obtain, one has to be content with approximate flows and approximate sensitivities. Again, all computational methods produce approximations to $\boldsymbol{U}_\alpha$ so that which method one uses should be determined by accuracy and cost considerations. Likewise, if one wants to use sensitivities to calculate approximate nearby flows, one again needs accurate sensitivities. In these respects, the sensitivity equation approach is probably better in most situations.

Despite this discussion, our goal here is not to apply flow sensitivities or even to critically compare methods for their determination. Rather, we want to discuss difficulties that arise in the computation of flow sensitivities for discontinuous flows by any method. We also note that adjoint methods can also be effectively used in an optimization setting for compressible flows (e.g., Refs. 16–18) and that, if many design parameters are in effect, these methods can be more efficient than sensitivity-based methods. However, the difficulties discussed in this paper for sensitivities are shared by adjoint variables.

III. Riemann Problem

The one-dimensional Riemann or shock tube problem from gas dynamics[19–22] will be used in the calculation of the sensitivities as it contains many troublesome aspects present in typical flow solutions, including shock waves, rarefaction waves, and contact discontinuities. In this problem, two gases of different pressures and densities are in a tube separated by a diaphragm. If the diaphragm is broken, the gas of higher pressure and density will flow into the gas of lower pressure and density. The Riemann problem is to calculate this flow as a function of time and space.

The one-dimensional time-dependent equations of gas dynamics can be written in conservation law form as

$$\boldsymbol{U}_t + \boldsymbol{F}(\boldsymbol{U})_x = 0 \tag{1}$$

where

$$\boldsymbol{U} = \begin{bmatrix} \rho \\ m \\ e \end{bmatrix}, \qquad \boldsymbol{F}(\boldsymbol{U}) = \begin{bmatrix} m \\ (m^2/\rho) + P \\ (m/\rho)(e+P) \end{bmatrix}$$

The variables are related by the equation of state $e = \rho\epsilon + \frac{1}{2}\rho u^2$, where $\epsilon = P/(\gamma - 1)\rho$. The equations can also be written in nonconservation law form as

$$\boldsymbol{U}_t + A(\boldsymbol{U})\boldsymbol{U}_x = 0 \tag{2}$$

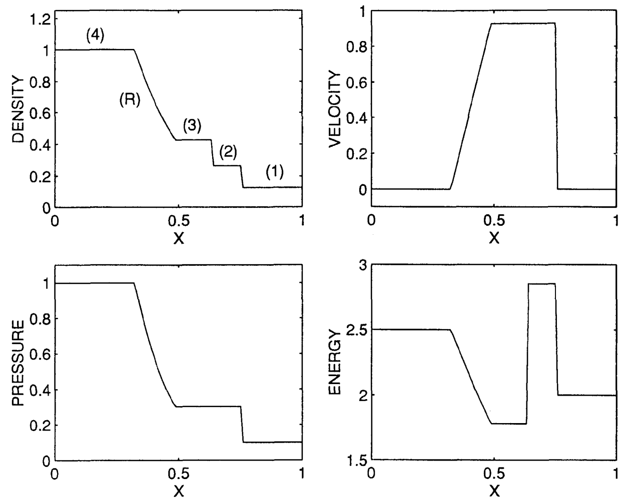

Fig. 1 Exact solution of the one-dimensional Riemann problem at t = 0.148.

where

$$A(U) = \begin{bmatrix} 0 & 1 & 0 \\ -(3-\gamma)(u^2/2) & (3-\gamma)u & \gamma - 1 \\ (\gamma-1)u^3 - (\gamma u e/\rho) & (\gamma e/\rho) - \frac{3}{2}(\gamma-1)u^2 & \gamma u \end{bmatrix}$$

The problem is defined on the region $\Omega = [-\infty, \infty] \times [0, T]$. Initially, both gases are at rest and are at different pressures and densities defined by $P_4 > P_1$, $\rho_4 > \rho_1$, and $u_4 = u_1 = 0$ with each P_j, ρ_j, and u_j defined on a different subregion. (Note: the subscript j refers to the region in which the variables are defined.) The exact initial conditions used in the calculations are $P_4 = \rho_4 = 1.0$, $P_1 = 0.1$, $\rho_1 = 0.125$, and $\gamma_j = 1.4$.

The solution of the one-dimensional Riemann problem has five distinct regions, as seen in Fig. 1: region (1), low-pressure and density region; region (2), area between shock and contact discontinuity region; region (3), area between contact discontinuity and rarefaction wave region; region (R), rarefaction wave and region; and region (4), high-pressure and density region. The exact solution can be solved for explicitly as a function of x and t in each region,[19,23] and for brevity it is not included here. The solution at time $t = 0.148$ and for $0 \le x \le 1$ is plotted in Fig. 1. The initial position of the diaphragm was $x = 0.5$.

IV. Exact Continuous Sensitivity of the Riemann Problem

Several methods for calculating flow sensitivities are considered by calculating the sensitivity of the flow with respect to a specific parameter. The parameter chosen is the initial high-pressure P_4. In the following sections the flow sensitivity with respect to P_4 will be calculated using finite difference quotients, the sensitivity equation method, and ADIFOR for a variety of numerical schemes. The exact continuous sensitivity can be calculated in each region from the explicit solution of the Riemann problem.[19,23] The solution of the one-dimensional Riemann problem has five distinct regions, as seen in Fig. 1. Hence, the solution can be differentiated in each region to calculate the exact continuous sensitivity of the flow in that region with respect to the variable P_4. Note that the differentiation is not across shocks or contact discontinuities. If the differentiation had occurred across these phenomena, then a δ-function would result at the discontinuity. In either case, the exact continuous sensitivity should hold everywhere in the domain except at the point where th discontinuity occurs. After differentiation, flow sensitivities witl respect to P_4 at a time t and a position x are given later. The region are the same as those defined for the explicit flow solution: in regio (4), the sensitivity variables are given by $P_4' = 1$, $\rho_4' = 0$, an $u_4' = 0$, where

$$\begin{bmatrix} P_i' \\ \rho_i' \\ u_i' \end{bmatrix} = \begin{bmatrix} \dfrac{\partial P_i}{\partial P_4} \\ \dfrac{\partial \rho_i}{\partial P_4} \\ \dfrac{\partial u_i}{\partial P_4} \end{bmatrix}$$

Likewise, in region (1), the sensitivity variables are given b $P_1' = 0$, $\rho_1' = 0$, and $u_1' = 0$. The sensitivity variables $(\partial e_i/\partial P_4) =$ e_i' and $(\partial m_i/\partial P_4) = m_i'$ can be solved for from the following equa tions, which depend on the flow solution:

$$e_i' = [P_i'/(\gamma_i + 1)] + \tfrac{1}{2}\rho_i' u_i^2 + \rho_i u_i u_i' \qquad (3$$

$$m_i' = \rho_i' u_i + \rho_i u_i' \qquad (4$$

Across the contact discontinuity the pressure and velocity ar continuous so that the sensitivity variables $P_2' = P_3'$ and $u_2' =$ u_3'. The equation for P_2' is found by differentiating the implici equation

$$\frac{P_4}{P_1} = \frac{P_2}{P_1}\left\{1 - \frac{(\gamma_4 - 1)(a_1/a_4)[(P_2/P_1) - 1]}{\sqrt{2\gamma_1}\sqrt{2\gamma_1 + (\gamma_1 + 1)[(P_2/P_1) - 1]}}\right\}^{-2\gamma_4/(\gamma_4 - 1)}$$

for P_2 with respect to P_4 and solving for P_2'. This equation is no considered here for lack of space, but it can be derived using a littl calculus and is explicit in P_2'. The other variables, ρ_2', ρ_3', and u_3' are given in terms of P_2' and the flow variables by

$$\rho_2' = \rho_1\left(\frac{P_2'}{P_1}\right)\left\{\frac{1 + [(\gamma_1 - 1)/(\gamma_1 + 1)](P_1/P_2)}{1 + [(\gamma_1 - 1)/(\gamma_1 + 1)](P_2/P_1)}\right\} + \rho_1\left(\frac{P_2}{P_1}\right)\left(\frac{\gamma_1 - 1}{\gamma_1 + 1}\right)$$
$$\times\left(\frac{[(-P_1/P_2^2)P_2']\{1 + [(\gamma_1 - 1)/(\gamma_1 + 1)(P_2/P_1)]\} - \{1 + [(\gamma_1 - 1)/(\gamma_1 + 1)(P_1/P_2)]\}(P_2'/P_1)}{\{1 + [(\gamma_1 - 1)/(\gamma_1 + 1)](P_2/P_1)\}^2}\right) \qquad (5$$

$$\rho_3' = \rho_4\left(\frac{1}{\gamma_4}\right)\left(\frac{P_3}{P_4}\right)^{(1-\gamma_4)/\gamma_4}\left(\frac{P_3'P_4 - P_3}{P_4^2}\right) \qquad (6$$

$$u_3' = \frac{2a_4'}{\gamma_4 - 1}\left[1 - \left(\frac{P_3}{P_4}\right)^{(\gamma_4-1)/2\gamma_4}\right]$$
$$-\left(\frac{a_4}{\gamma_4}\right)\left(\frac{P_3}{P_4}\right)^{(-\gamma_4-1)/2\gamma_4}\left(\frac{P_3'P_4 - P_3}{P_4^2}\right) \qquad (7$$

with $a_4' = \frac{1}{2}(\gamma_4 P_4/\rho_4)^{-1/2}(\gamma_4/\rho_4)$ and $a_i = \sqrt{(\gamma_i P_i/\rho_i)}$.

In the rarefaction wave, region (R), the sensitivity variables P_R', ρ_R', and u_R' are

$$P_R' = \left(1 + \frac{\gamma_4 - 1}{2}\frac{u_R}{a_4}\right)^{2\gamma_4/(\gamma_4 - 1)}$$
$$+ P_4\gamma_4\left(1 + \frac{\gamma_4 - 1}{2}\frac{u_R}{a_4}\right)^{(2\gamma_4+1)/(\gamma_4-1)}\left(\frac{u_R'a_4 - u_R a_4'}{a_4^2}\right) \qquad (8)$$

$$\rho_R' = \left(1 + \frac{\gamma_4 - 1}{2}\frac{u_R}{a_4}\right)^{(3-\gamma_4)/(\gamma_4-1)}\left(\frac{u_R'a_4 - u_R a_4'}{a_4^2}\right) \qquad (9)$$

$$u_R' = 2a_4'/(\gamma_4 + 1) \qquad (10)$$

The exact flow sensitivities with respect to the parameter P_4 can be seen in Fig. 2 at time $t = 0.148$ and for $0 \le x \le 1$. Note the discontinuities at the boundaries of the rarefaction wave region.

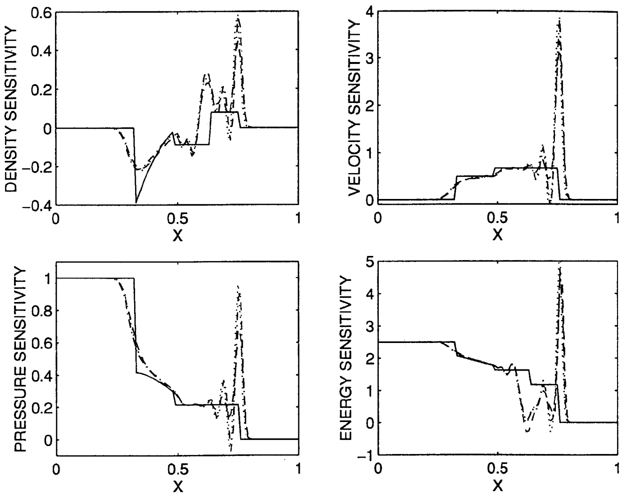

Fig. 2 Comparison of the three different sensitivity calculation methods using the Lax–Wendroff numerical scheme vs the exact continuous sensitivity on a fine grid: · · · ·, ADIFOR sensitivity; -·-·-·, finite difference sensitivity; – – –, sensitivity equation method sensitivity; and ——, exact continuous sensitivity.

V. Continuous Sensitivity Equations

The continuous sensitivity equations for the sensitivity equation method are derived by differentiating the original flow equations, Eq. (1), and initial conditions with respect to P_4. The continuous sensitivity equations can be written in conservation law form as

$$S_t + [G(U, S)]_x = 0 \tag{11}$$

where

$$G(U,S) = \frac{\partial F}{\partial P_4}(U) = \begin{bmatrix} m' \\ (2mm'/\rho) - (m^2/\rho^2)\rho' + P' \\ [(m'/\rho) - (m/\rho^2)\rho'](e+P) + (m/\rho)(e'+P') \end{bmatrix}$$

$$S = \begin{bmatrix} \rho' = \dfrac{\partial \rho}{\partial P_4} \\ m' = \dfrac{\partial m}{\partial P_4} \\ e' = \dfrac{\partial e}{\partial P_4} \end{bmatrix}$$

and where $m' = \rho' u + \rho u'$ and $e' = [P'/(\gamma - 1)] + \frac{1}{2}\rho' u^2 + \rho u u'$. The initial conditions for the system are given by

$$S(x,0) = f(x) = \begin{cases} \begin{bmatrix} 0 \\ 0 \\ 1/(\gamma_4 - 1) \end{bmatrix} & x \le 0 \\ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} & x > 0 \end{cases} \tag{12}$$

Note that, as is discussed in Sec. VII, the sensitivity equations, Eq. (11), only hold within each of the regions 1–4 and R but do not hold across the shock, the contact discontinuity, or even the two ends of the rarefaction wave.

VI. Numerical Methods

The Riemann problem and the continuous sensitivity equations are solved using three different numerical schemes. The first is a two-step Lax–Wendroff finite difference scheme described in Ref. 22:

$$U_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \tfrac{1}{2}\left(U_{i+1}^n + U_i^n\right) - (\Delta t/2\Delta x)\left(F_{i+1}^n - F_i^n\right)$$
$$\hat{U}_i^{n+1} = U_i^n - (\Delta t/\Delta x)\left(F_{i+\frac{1}{2}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) \tag{13}$$

The second is the Godunov finite difference scheme described in Ref. 22:

$$U_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \tfrac{1}{2}\left(U_{i+1}^n + U_i^n\right) - (\Delta t/\Delta x)\left(F_{i+1}^n - F_i^n\right)$$
$$\hat{U}_i^{n+1} = U_i^n - (\Delta t/\Delta x)\left(F_{i+\frac{1}{2}}^{n+\frac{1}{2}} - F_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) \tag{14}$$

Both the two-step Lax–Wendroff scheme and the Godunov scheme have the postprocessing artificial viscosity term of Lapidus[22] added to the solution. Let $\hat{U}_i^{n+1}$ be the approximate solution at the next time step. The solution is then replaced by

$$U_i^{n+1} = \hat{U}_i^{n+1} + (\nu\Delta t/\Delta x)\Delta'\left[\left|\Delta'\hat{U}_{i+1}^{n+1}\right| \cdot \Delta'\hat{U}_{i+1}^{n+1}\right] \tag{15}$$

where $\Delta'\hat{U}_i^n = \hat{U}_i^n - \hat{U}_{i-1}^n$, and ν is an adjustable constant.

The final scheme is the Roe scheme as described in Ref. 21:

$$U_i^{n+1} = U_i^n - (\Delta t/\Delta x)\left(F_{i+\frac{1}{2}}^* - F_{i-\frac{1}{2}}^*\right) \tag{16}$$

where

$$F^* = \frac{1}{2}(F_i + F_{i+1}) - \frac{1}{2}\sum_j |\bar{\lambda}_j| \partial w_j \bar{r}_j$$

and where $\bar{\lambda}_j$ and $\bar{r}_j$ are the eigenvalues and eigenvectors of the Roe-averaged Jacobian matrix $\bar{A}(U_i, U_{i+1})$. The sonic entropy fix of Harten and Hyman[21] is added to the Roe scheme as well as the second-order superbee flux-limiter method. The Roe calculations were performed using CLAWPACK routines.

The preceding numerical schemes are described in terms of the original Riemann problem. For the continuous sensitivity equations, using the Lax–Wendroff and Godunov schemes, U is replaced by S and F is replaced by G. The Roe scheme for the continuous sensitivity requires a small modification. The nonconservation law form of the continuous sensitivity equations is given in Eq. (17),

$$S_t + A(U)S_x = -A(U)_x S \tag{17}$$

where $A(U)$ is the same flux Jacobian as in the flow equations. The implementation of the Roe scheme for the continuous sensitivity equations tries to preserve as much of the original work as possible. Hence, the continuous flow equations for the Roe scheme are treated as a conservation law with a source term. This can be solved using a splitting approach, in which one alternates between solving the homogeneous equation

$$S_t + A(U)S_x = 0 \tag{18}$$

and the equation

$$S_t = -A(U)_x S \tag{19}$$

The method employed uses Strang splitting,[24] where a single time step Δt of Eq. (17) is solved by first solving Eq. (19) over half a time step length $\Delta t/2$, then using these results for solving Eq. (18) over a full time step, and finally solving Eq. (19) over a half time step. This method is appealing because Eq. (18) is identical to the non-conservation form of the Euler equations, and thus it uses the same Roe-averaged Jacobian matrix as the flow equations. The source equation, Eq. (19), is solved using the following discretization:

$$S_i^{n+\frac{1}{2}} = S_i^n - (\Delta t/\Delta x)\left[A\left(U_i^n\right) - A\left(U_{i-1}^n\right)\right] \tag{20}$$

The Roe scheme for the continuous sensitivity equations was calculated using modified versions of CLAWPACK routines.

The continuous sensitivity equations for high-speed flows will be linear hyperbolic equations with discontinuous coefficients. There seems to be little literature on these types of equations. LeVeque

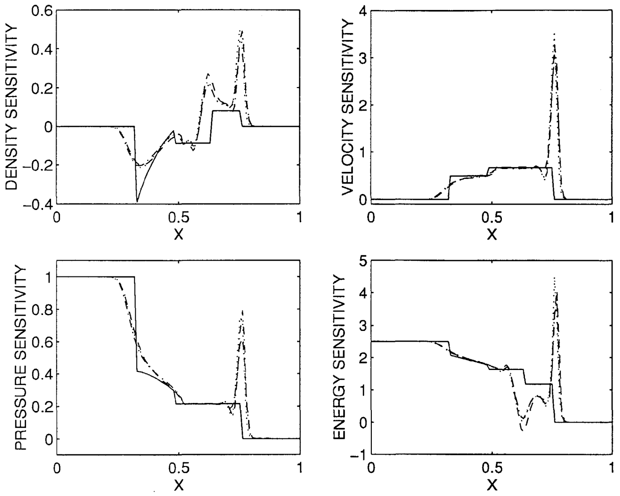

Fig. 3 Comparison of the three different sensitivity calculation methods using the Godunov numerical scheme vs the exact continuous sensitivity on a fine grid: · · · ·, ADIFOR sensitivity; -·-·-, finite difference sensitivity; – – –, sensitivity equation method sensitivity; and ——, exact continuous sensitivity.

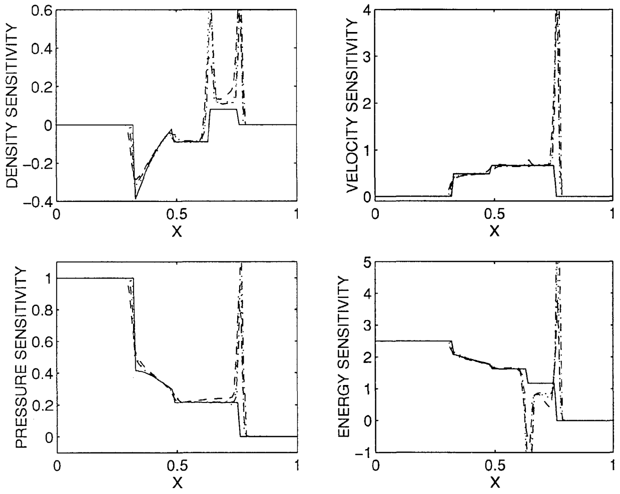

Fig. 4 Comparison of the three different sensitivity calculation methods using the Roe numerical scheme vs the exact continuous sensitivity on a fine grid: · · · ·, ADIFOR sensitivity; -·-·-, finite difference sensitivity; – – –, sensitivity equation method sensitivity; and ——, exact continuous sensitivity.

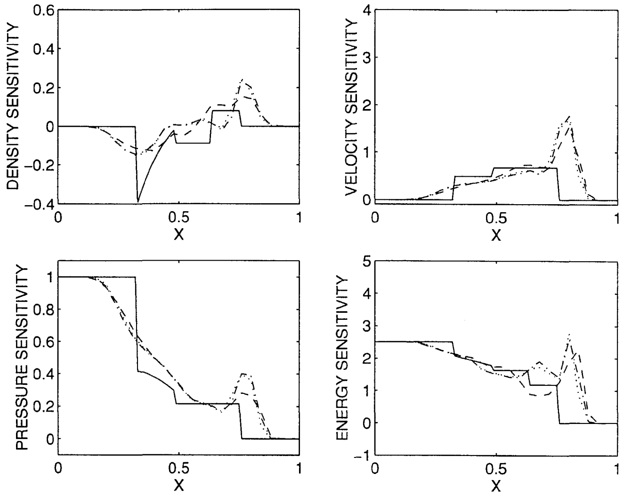

Fig. 5 Comparison of the three different sensitivity calculation methods using the Lax-Wendroff numerical scheme vs the exact continuous sensitivity on a coarse grid: · · · ·, ADIFOR sensitivity; -·-·-, finite difference sensitivity; – – –, sensitivity equation method sensitivity; and ——, exact continuous sensitivity.

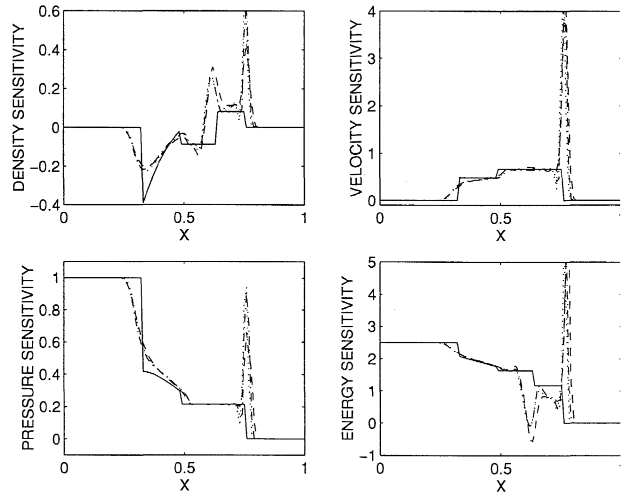

Fig. 6 Comparison of the three different sensitivity calculation methods using the Lax-Wendroff numerical scheme vs the exact continuous sensitivity using a larger Δt: · · · ·, ADIFOR sensitivity; -·-·-, finite difference sensitivity; – – –, sensitivity equation method sensitivity; and ——, exact continuous sensitivity.

and Zhang[25] present one approach, but assumptions require that the discontinuity is at a fixed location throughout time and does not apply to the Riemann problem.

The sensitivities have been calculated using finite differences, ADIFOR, and the sensitivity equation method using the three numerical schemes described earlier. The spatial grid size was $\Delta x = 0.01$, and the temporal grid size was $\Delta t = 0.001$. The numerical solutions of these sensitivities are given in Figs. 2–4 vs the exact continuous sensitivity. The graphs are printed on identical scales, and hence the spikes for the Roe scheme go off of the graph.

Figures 2–4 clearly show little difference between the three different sensitivity calculations. Thus, the method or numerical scheme may not be that important, and the easiest and cheapest method should be used. But there are still many problems with the sensitivities in the presence of flow discontinuities. Another important question is how the grid spacing affects the sensitivity calculation methods. In many applications such a fine grid is infeasible; for this reason, the Lax–Wendroff sensitivities are given in Fig. 5 vs the exact continuous sensitivities for a coarse grid of $\Delta t = 0.016444$ and $\Delta x = 0.04$. The discontinuities have an even larger effect for the coarse grid as the δ-functions and jump discontinuities smear out over a larger area and most of the solution structure is lost.

There are noticeable oscillations in front of the shock positior in the flow sensitivities using the Lax–Wendroff method on a fine grid. This is due to the oscillations that occur in the flow solutior before the shock as expected with the Lax–Wendroff method[21] ir the prescence of discontinuities. In fairness, better results can be achieved using a larger time step. The Lax–Wendroff sensitivities are shown in Fig. 6 vs the exact continuous sensitivity using $\Delta t = 0.004$ and $\Delta x = 0.01$. Note the lack of large oscillation in front of the shock position.

Clearly, the sensitivity calculation methods have problems wherever there is a discontinuity in the flow or in the sensitivity. These reasons are discussed in Sec. VII.

VII. Flow Sensitivities and Discontinuities

A. Shock Waves

The calculation of flow sensitivities in the presence of shock waves is a difficult enterprise. In the sensitivity equation method, the automatic differentiation method, and the finite difference method one must deal with the discontinuities occurring at the shock wave.

Suppose that the flow is characterized by a single parameter α. Then because the flow is described by a one-dimensional equation the flow may be viewed as a function of x and α, i.e., $U(x, \alpha)$. (All references to the time t have been omitted as it is assumed

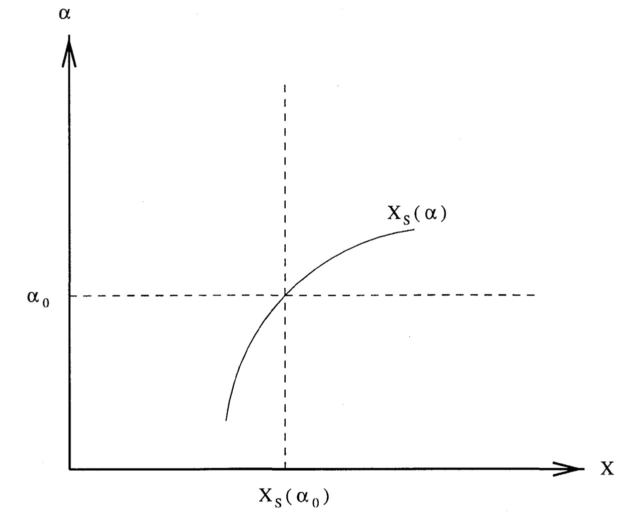

Fig. 7 Shock wave in (x, α) space. Flow variables are discontinuous when one crosses the shock wave $x_s(\alpha)$ at the point $[x_s(\alpha_0), \alpha_0]$ along either the horizontal or vertical dashed lines.

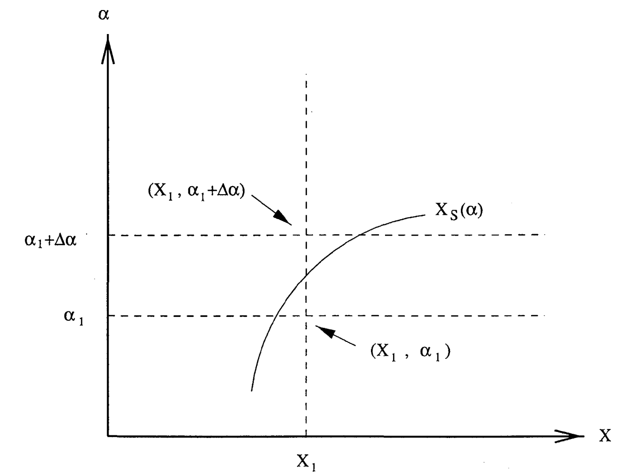

Fig. 8 Points (x_1, α_1) and $(x_1, \alpha_1 + \triangle\alpha)$ are on opposite sides of the shock wave. The variables at the two points differ significantly even if the two points are close together, i.e., even if $\triangle\alpha$ is small.

that all calculations are performed at a specific time t_0.) For a flow simulation, one would pick a particular value of α_0 for the parameter and then proceed to determine $\boldsymbol{U}$ as a function of x, i.e., $\boldsymbol{U}(x; \alpha_0)$. The location of the shock wave is denoted by x_s. In general, if the value of the parameter is changed, the location of the shock wave change and so the shock location is a function of the parameter $x_s = x_s(\alpha)$, and thus at a particular value α_0 the shock location is given by $x_s(\alpha_0)$, as sketched in Fig. 7. Thus, for a fixed value of the parameter $\alpha = \alpha_0$, the flow variable $\boldsymbol{U}(x; \alpha_0)$ is a discontinuous function of x and certainly cannot be differentiated with respect to x at $x_s(\alpha_0)$. Likewise, if the value of x is fixed to, say, $x = x_0$, then for at least some x_0, $\boldsymbol{U}(x_0, \alpha)$, viewed as a function of α, is discontinuous and hence not differentiable with respect to α at $x_s(\alpha) = x_0$.

The conclusion that can be drawn from the preceding discussion is that, strictly speaking, flow sensitivity derivatives do not exist at shock waves in much the same way that spatial and temporal flow derivatives do not exist at those locations. In the calculation of flow sensitivities by all three numerical approaches, the presence of shock waves has been ignored; e.g., the same algorithm has been applied at points in (x, α) space where a shock wave is present as was applied at points where the flow is smooth. As a result, flow sensitivities with large spikes at the shock are obtained; these spikes approximate the δ-function that the exact flow sensitivities contain at that location.

To see how these spikes arise, consider the difference quotient approach to approximating sensitivities. The flow is computed at (x_1, α_1) and at $(x_1, \alpha_1 + \Delta\alpha)$, and the flow sensitivity is approximated by

$$\frac{\partial \boldsymbol{U}}{\partial \alpha} \approx \frac{\boldsymbol{U}(x_1, \alpha_1 + \Delta\alpha) - \boldsymbol{U}(x_1, \alpha_1)}{\Delta\alpha} \tag{21}$$

Of course, if the flow is smooth and $\Delta\alpha$ is small, then both the numerator and the denominator in Eq. (21) will be small, and in fact, as $\Delta\alpha \to 0$, both approach zero in such a way that their ratio converges to $\partial \boldsymbol{U}/\partial\alpha(x_1, \alpha_1)$. Now, suppose that the points (x_1, α_1) and $(x_1, \alpha_1 + \Delta\alpha)$ lie on opposite sides of the shock wave as in Fig. 8. Then even if $\Delta\alpha$ is small, the numerator in Eq. (21) is relatively large. Hence, the solution of the finite difference sensitivity is large, and a spike occurs when differencing across a shock.

In the sensitivity equation approach, the same spikes develop. To understand this, consider Eq. (1). Again suppose one parameter α determines the flow, $\boldsymbol{U}(x, t; \alpha)$. The equation for the sensitivity $\boldsymbol{S} = \partial \boldsymbol{U}/\partial\alpha$ is determined by differentiating Eq. (1) with respect to α:

$$0 = \frac{\partial}{\partial\alpha}\left[\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{U})}{\partial x}\right] \tag{22}$$

$$0 = \frac{\partial^2 \boldsymbol{U}}{\partial\alpha\partial t} + \frac{\partial^2 \boldsymbol{F}(\boldsymbol{U})}{\partial\alpha\partial x} \tag{23}$$

$$0 = \frac{\partial}{\partial t}\left(\frac{\partial \boldsymbol{U}}{\partial\alpha}\right) + \frac{\partial}{\partial x}\left[\frac{\partial \boldsymbol{F}(\boldsymbol{U})}{\partial\alpha}\right] \tag{24}$$

$$0 = \frac{\partial \boldsymbol{S}}{\partial t} + \frac{\partial}{\partial x}\boldsymbol{G}(\boldsymbol{U}, \boldsymbol{S}) \tag{25}$$

where the flux function $\boldsymbol{G}(\boldsymbol{U}, \boldsymbol{S})$ of the sensitivity equation is defined by

$$\boldsymbol{G}(\boldsymbol{U}, \boldsymbol{S}) = \frac{\partial \boldsymbol{F}(\boldsymbol{U})}{\partial\alpha} = \frac{\mathrm{d}\boldsymbol{F}}{\mathrm{d}\boldsymbol{U}}(\boldsymbol{U})\boldsymbol{S}$$

In calculating this equation, note that the orders of differentiation have been interchanged. In smooth regions of the flow, there is no difficulty in interchanging derivatives; however, at a shock wave the derivation embodied in Eq. (24) is not allowable due to the nonexistence of the appropriate derivatives at that location. Thus, one should not use the flux function $\boldsymbol{G}$ as defined earlier.

B. Contact Discontinuities

Contact discontinuities are another source of error in the sensitivity calculations. Across a contact discontinuity, the velocity u and the pressure P are continuous, whereas the density ρ and hence other conserved quantities experience a jump discontinuity. Thus, for the conserved quantities the same problems, as are described earlier, arise, and spikes arise in the conserved quantities sensitivities at the contact discontinuity.

C. Rarefaction Waves

The final source of error considered here is the rarefaction wave. Previously, it has been believed that because the rarefaction wave is continuous, then the sensitivities will also be continuous and of little problem computationally. Although the sensitivities are continuous in the rarefaction wave, they still present computational difficulties. A new problem has arisen at the boundaries of the rarefaction wave region. The flow sensitivities introduce a jump condition at both ends of the wave, making it difficult to capture the correct sensitivity. The numerical methods used are designed to correctly capture jump discontinuities for the flow, and it would be reasonable to expect a similar behavior for the flow sensitivities. The problem is that the approximate flow solution is used to calculate the flow sensitivities. Hence, a second level approximation is going on, which makes it difficult to capture the jump discontinuity. In effect, a smearing of the discontinuity takes place at both ends of the rarefaction wave. This is very noticeable in the ρ' variable. For more accurate solutions, this must be dealt with numerically. One possible method is to refine the grid. This will lead to more accurate sensitivities in the rarefaction wave region but will greatly increase the cost of the method.

VIII. Conclusion

Flow sensitivities have applications not only in flow optimizations but also in the calculation of perturbed flows and as informational tools. Flow sensitivities are currently being used in flow optimizations, but to be a useful tool in the other contexts many improvements are needed. One of these improvements is in the area of calculation of sensitivities in discontinuous flows. Shocks, contact discontinuities, and even rarefaction waves, even though they are not discontinuous, cause major difficulties in these calculations. Now that the problems have been isolated and an understanding has been gained, the next step is to compute correct flow sensitivities. If this can be done in an efficient manner, then the applications to optimization, nearby flows, and other settings are numerous.

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