



Numerical and theoretical considerations for sensitivity calculation of discontinuous flow[☆]

Chris Homescu, I.M. Navon*

Department of Mathematics and School of Computational Science and Information Technology, Florida State University, Tallahassee, FL 32306, USA

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This paper is dedicated to J.L. Lions in deep homage

Abstract

Linearization of 1-D Euler equations about a discontinuous solution is discussed from both the theoretical and numerical point of view. Estimates for the norm of the solution of the linearized system are shown to be valid for the case presented. Numerically, the linearization is performed following the guidelines of tangent linear model and sensitivities with respect to a flow parameter are computed, being in better agreement with the analytical value when compared with previously reported numerical results.

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1. Introduction

Sensitivities (which are derivatives of the variables or cost functionals that describe the model with respect to parameters that determine the behavior of the model, e.g., initial conditions, boundary conditions, shape parameters, etc.) were extensively studied in the last decades for problems involving continuous functions. Research was performed also in the presence of discontinuities but many questions in this area remain yet unanswered.

Sensitivity analysis in the case of a model with discontinuities was applied in areas like fluid dynamics, aerodynamics, chemistry, financial analysis, meteorology or environmental studies, to name but a few.

Studies include shape optimization for fluids [2,18,23,16], noise analysis and optimization of electronic circuits [19], control of contaminant releases in rivers [20], control of water movement through systems of irrigation canals [21], shallow water wave control [22], aeroelastic analysis [7], shock sensitivity evaluations of dynamic financial strategies [9] and meteorological applications [25].

Theoretical and computational aspects of sensitivity calculation in the presence of discontinuities were also presented by Ulbrich [24], Cliff et al. [3], Godlewski and Raviart [8], Bouchut and James [1] and DiCesare and Pironneau [6].

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* Corresponding author.

E-mail addresses: chome@math.fsu.edu (C. Homescu), navon@csit.fsu.edu (I.M. Navon).

Numerical sensitivities were computed by Narducci et al. [17] for optimization of duct flow with a shock using quasi-one-dimensional Euler equations. In their research they employed continuous (*differentiate-then-discretize*) and discrete (*discretize-then-differentiate*) methods to compute the design sensitivities. The continuous method requires analytical expressions for the derivatives of the velocity and shock location with respect to the design variables derived from the governing equations and the shock jump conditions (the difference between direct and adjoint method in this case is that the adjoint method avoids computing these derivatives directly). For the discrete method a coordinate-straining approach with a shock penalty was employed (to avoid difficulties caused by the presence of nonsmooth functions).

For the same problem as Narducci et al. (quasi-one-dimensional duct flow) Cliff et al. [3] introduced the shock location as an explicit variable which allowed one to fit the shock and yielded a problem with sufficiently smoothed functions.

Cliff et al. [4] carried out sensitivity calculations for the 1D Euler system. No numerical calculations were performed however.

Our research is focused on the numerical computation of flow sensitivities with respect to an initial flow parameter for the shock-tube problem (1-D Riemann problem described by Euler equations).

We chose the discrete (*discretize-then-differentiate*) approach which in our opinion is more suitable than the continuous approach for flows with discontinuities.

2. Model formulation

We chose to perform linearization of 1-D Euler equations and sensitivity computation for this discontinuous flow, since the one-dimensional shock-tube problem from gas dynamics contains many potential “troublesome” characteristics of a flow with discontinuities, including shock waves, rarefaction waves and contact discontinuities.

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

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = 0, \quad (1)$$

where

$$\mathbf{U} = \begin{bmatrix} \rho \\ m \\ e \end{bmatrix}, \quad \mathbf{F}(\mathbf{U}) = \begin{bmatrix} m \\ \frac{m^2}{\rho} + P \\ \left(\frac{m}{\rho}\right)(e + P) \end{bmatrix} \quad (2)$$

and where ρ is the density, u is the velocity, $m = \rho u$ is momentum, P is the pressure and e is the internal energy per unit volume. The variables are related by $e = \rho\varepsilon + \frac{1}{2}\rho u^2$, where $\varepsilon = P/(\gamma - 1)\rho$ is the internal energy per internal mass with γ the ratio of specific heats (which is taken to be 1.4).

We study the Riemann problem which can be described as follows. There is a shock tube with two gases separated by a membrane. Initially, both gases are at rest and are at different pressures and densities defined by $P_4 > P_1$, $\rho_4 > \rho_1$, and $u_4 > u_1$ where the subscript refers to the region in which the variables are defined (initially region 4 at the left of the membrane and region 1 is at the right of the membrane; afterwards region 4 is first region from the left boundary and region 1 is the first region from the right boundary (see Fig. 1).

The exact solution can be found explicitly as a function of x and t (see [14]) and its plot (numerical solution versus analytical solution) is shown in Fig. 1. The solution has several distinct regions: a region of low pressure and density; an area between shock and contact discontinuity; an area between contact discontinuity and rarefaction wave; a rarefaction wave and a region of high pressure and density.

3. Tangent linear system approach for the sensitivity computation

We consider a symbolic form for a time-dependent system of equations

$$\frac{\partial \mathbf{X}}{\partial t} = N(\mathbf{X}). \quad (3)$$

Then the perturbed solution ($\mathbf{X}(t) + \delta\mathbf{X}(t)$) satisfies the equation

$$\begin{aligned} \frac{\partial(\mathbf{X}(t) + \delta\mathbf{X}(t))}{\partial t} &= N(\mathbf{X}(t) + \delta\mathbf{X}(t)) \\ &= N(\mathbf{X}(t)) + \frac{\partial N}{\partial \mathbf{X}}(\mathbf{X}(t))\delta\mathbf{X}(t) + O(\delta\mathbf{X}(t)), \end{aligned}$$

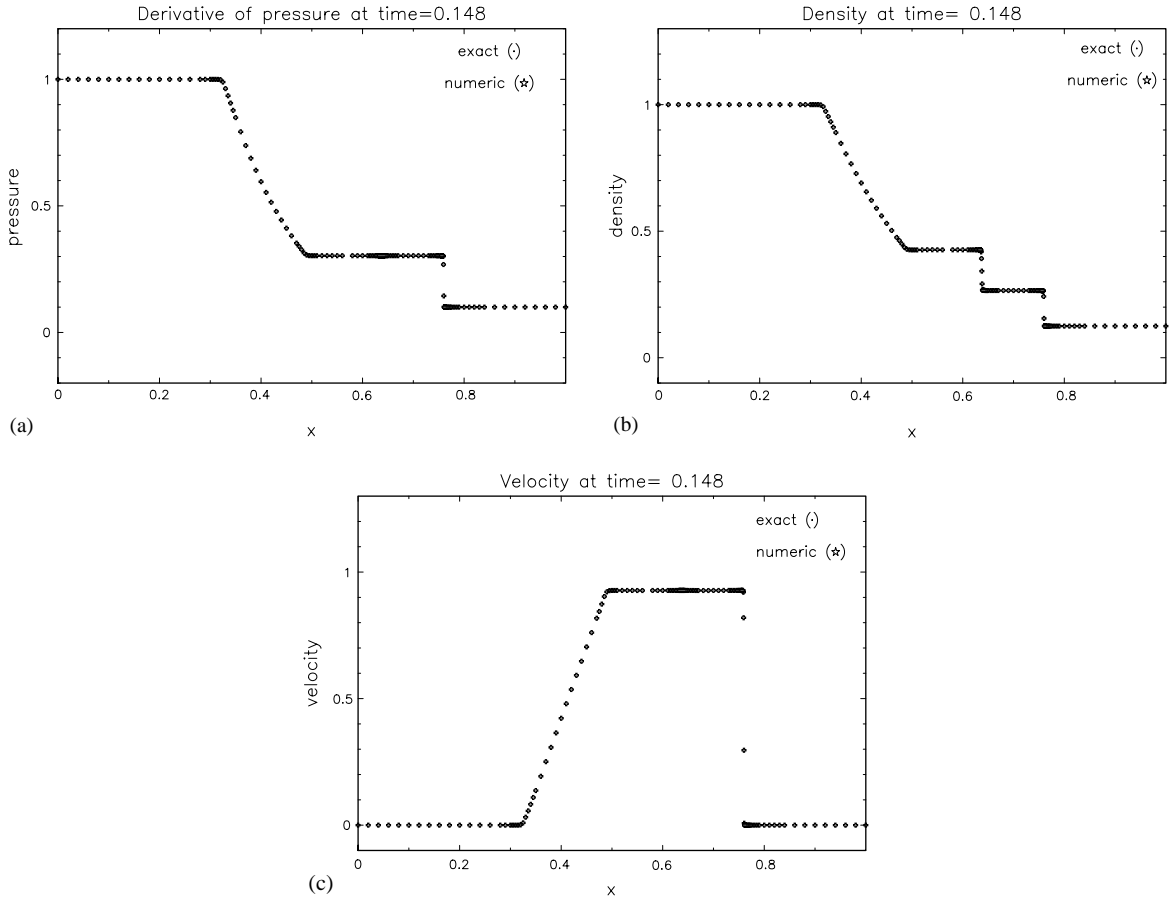


Fig. 1. Exact solution of the shock-tube problem: numerical and exact values for (a) pressure, (b) density and (c) velocity.

where $\partial N / \partial \mathbf{X}$ is the Jacobian of the nonlinear function N with respect to the variables \mathbf{X} . Upon retaining only the first-order terms in $\delta \mathbf{X}$ the previous equation becomes

$$\frac{\partial \delta \mathbf{X}(t)}{\partial t} = \frac{\partial N}{\partial \mathbf{X}}(\mathbf{X}(t)) \delta \mathbf{X}(t). \quad (4)$$

To determine the sensitivity with respect to a parameter α we differentiate Eq. (3). Assuming that we can interchange the order of differentiation we obtain

$$\frac{\partial}{\partial t} \left(\frac{\partial \mathbf{X}}{\partial \alpha} \right) = \frac{\partial N(\mathbf{X})}{\partial \mathbf{X}} \frac{\partial \mathbf{X}}{\partial \alpha}, \quad (5)$$

which implies that the sensitivity $\partial \mathbf{X} / \partial \alpha$ with respect to the parameter α satisfies also tangent linear equation (4). This provides the rationale for the numerical

computation of the sensitivity using the tangent linear model.

4. Linearization of the Euler equations

The following derivation follows Godlewski and Raviart [8].

Given a solution of (1), called *basic solution*, we study the behavior in time of solutions of the linear hyperbolic system obtained by linearizing (1) at the basic solution. Since the basic solution is discontinuous the linearized system has discontinuous coefficients and it is not well posed in any class of functions. The solution of the linearized system consists of the sum of a function and a measure caused by the discontinuity of the basic solution.

Let $\mathbf{U} = \mathbf{U}(x, t)$ be the basic solution and

$$\mathbf{U}^\varepsilon = \mathbf{U}(x, t) + \varepsilon \mathbf{V}(x, t),$$

$$\mathbf{U}^\varepsilon(x, 0) = \mathbf{U}(x, 0) + \varepsilon \mathbf{V}(x, 0) = \mathbf{U}_0(x) + \varepsilon \mathbf{V}_0(x)$$

with $\varepsilon > 0$ a small parameter.

The first order perturbation $\mathbf{V} = \mathbf{V}(x, t)$ is solution of the linearized problem

$$\begin{aligned} \frac{\partial \mathbf{V}}{\partial t} + \frac{\partial}{\partial x}(\mathbf{J}(\mathbf{U})\mathbf{V}) &= 0, \\ \mathbf{V}(x, 0) &= \mathbf{V}_0(x), \end{aligned} \quad (6)$$

where $\mathbf{J}(\mathbf{U})$ denote the Jacobian of $\mathbf{F}(\mathbf{U})$.

The basic solution \mathbf{U} presents a discontinuity along the line $\mathbf{L} = \{(x, t), x = \Phi(t), t \geq 0\}$ where the function $\Phi(t)$ is determined by the location of the shock (in our case

$$\Phi(t) = \left(\frac{\gamma P_1}{\rho_1}\right)^{1/2} \left(\frac{\gamma - 1}{2\gamma} + \frac{\gamma + 1}{2\gamma} \frac{P_2}{P_1}\right)^{1/2} + x_0,$$

where the subscript refers to the region in which the variables are defined and x_0 is the initial position of the diaphragm (at $t = 0$)).

\mathbf{U} presents at most weak discontinuities outside the line \mathbf{L} . For t small enough the problem retains the same characteristics but the perturbed solution \mathbf{U}^ε presents a discontinuity along a different line $\mathbf{L}^\varepsilon = \{(x, t), x = \Phi^\varepsilon(t) = \Phi(t) + \varepsilon \Psi(t), t \geq 0\}$ and at most weak discontinuities outside \mathbf{L}^ε .

We introduce the equation of the front of the discontinuities as one of the unknowns and we use a change of variables to reduce the problem to a fixed domain:

$$\hat{x} = x - \Phi^\varepsilon(t), \quad (7)$$

$$\hat{\mathbf{U}}^\varepsilon(\hat{x}, t) = \mathbf{U}^\varepsilon(\hat{x} + \Phi^\varepsilon(t), t). \quad (8)$$

The function \mathbf{U} is now discontinuous along the fixed line $\hat{x} = 0$ and is the solution of the Cauchy problem

$$\begin{aligned} \frac{\partial \hat{\mathbf{U}}^\varepsilon}{\partial t} + \frac{\partial}{\partial \hat{x}}(F(\hat{\mathbf{U}}^\varepsilon) - \frac{\partial \Phi^\varepsilon}{\partial t} \hat{\mathbf{U}}) &= 0, \\ \hat{\mathbf{U}}^\varepsilon(\hat{x}, 0) &= \mathbf{U}_0(\hat{x} + \Phi^\varepsilon(0)) + \varepsilon \mathbf{V}_0(\hat{x} + \Phi^\varepsilon(0)). \end{aligned} \quad (9)$$

Moreover $\hat{\mathbf{U}}^\varepsilon$ satisfies the Rankine–Hugoniot jump relations across $\hat{x} = 0$

$$[F(\hat{\mathbf{U}}^\varepsilon)] = \frac{\partial \Phi^\varepsilon}{\partial t} [\hat{\mathbf{U}}^\varepsilon]. \quad (10)$$

Recalling that

$$\hat{\mathbf{U}}(\hat{x}, t) = \mathbf{U}(\hat{x} + \Phi(t), t),$$

$$\hat{\mathbf{U}}^\varepsilon = \hat{\mathbf{U}} + \varepsilon \hat{\mathbf{U}} + \dots,$$

$$\Phi^\varepsilon = \Phi + \varepsilon \Psi.$$

We obtain that the pair $(\hat{\mathbf{V}}, \Psi)$ satisfies the linearized equations and the Rankine–Hugoniot relation:

$$\begin{aligned} \frac{\partial \hat{\mathbf{V}}}{\partial t} + \frac{\partial}{\partial \hat{x}} \left(\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \hat{\mathbf{V}} - \frac{\partial \Psi}{\partial t} \hat{\mathbf{U}} \right) &= 0, \\ \hat{\mathbf{V}}(\hat{x}, 0) &= \mathbf{V}_0(\hat{x}) + \Psi(0) \frac{d\mathbf{U}_0}{dx}(\hat{x}), \\ \left[\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \hat{\mathbf{V}} \right] &= \frac{\partial \Psi}{\partial t} [\hat{\mathbf{U}}]. \end{aligned} \quad (11)$$

Let us define $\bar{\mathbf{V}}(\hat{x}, t) = \hat{\mathbf{V}}(\hat{x}, t) - \Psi(t)(\partial \hat{\mathbf{U}} / \partial \hat{x})(\hat{x}, t)$. Then (see Appendix A) the pair $(\bar{\mathbf{V}}, \Psi)$ satisfies the following equations and jump condition:

$$\begin{aligned} \frac{\partial \bar{\mathbf{V}}}{\partial t} + \frac{\partial}{\partial \hat{x}} \left(\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \bar{\mathbf{V}} \right) &= 0, \\ \bar{\mathbf{V}}(\hat{x}, 0) &= \mathbf{V}_0(\hat{x}), \\ \left[\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \bar{\mathbf{V}} \right] &= \frac{\partial \Psi}{\partial t} [\hat{\mathbf{U}}] + \Psi \frac{\partial \hat{\mathbf{U}}}{\partial t}. \end{aligned} \quad (12)$$

Eqs. (12) have a unique solution [8]. The solution \mathbf{V} of the system (6) is defined as the sum of a function and a measure whose support is \mathbf{L}

$$\mathbf{V}(x, t) = \bar{\mathbf{V}}(x - \Phi(t), t) - \Psi[\mathbf{U}] \delta_{\mathbf{L}}, \quad (13)$$

where $\delta_{\mathbf{L}}$ is the Dirac measure with support \mathbf{L} .

5. L^2 estimates for the solution of the linearized Euler equations

L^2 estimates for the solution of the linearized system are obtained following the approach of Metivier [15].

Let $\Omega = \mathbf{R} \times [0, \infty]$ and $\omega = \{x = 0\}$ the boundary of Ω . We define $L^2_\eta = e^{\eta t} L^2$ and $H^1_\eta = e^{\eta t} H^1$ and in these spaces we consider the norms

$$\|u\|_{L^2_\eta}^2 = \int_{\Omega} e^{-2\eta t} |u(x)|^2 dx = \|e^{-\eta t} u\|_{L^2}^2,$$

$$\|u\|_{H^1_\eta}^2 = \|e^{-\eta t} u\|_{H^1}^2. \tag{14}$$

The solution $(\bar{\mathbf{V}}, \Psi) \in H^1_\eta(\Omega) \times H^1_\eta(\omega)$ of (12) satisfies the estimate

$$\eta \|\bar{\mathbf{V}}\|_{L^2_\eta(\Omega)}^2 + \|\bar{\mathbf{V}}|_{x=0}\|_{L^2_\eta(\omega)}^2 + \|\nabla \Psi\|_{L^2_\eta(\omega)}^2 \leq \frac{C}{\eta} \|e^{-\eta t} \mathbf{F}\|_0^2 \tag{15}$$

where C is a constant, $\eta \geq \eta_0$ with η_0 given and $\|u\|_{L^2_\eta} = \|e^{-\eta t} u\|_0$, with $\|u\|_0$ being the usual norm in L^2 .

6. Numerical considerations

To solve the Riemann problem we chose a code written by Li [13] which employs a method of adaptive

mesh refinement in conjunction with a Riemann solver of Roe-type [12]. The numerical solution is in very good agreement with the analytical solution and this eliminates a major source of errors in the numerical computation of the sensitivities.

We want to emphasize that one cannot differentiate the flow across the shock or the contact discontinuity since the flow is not continuous there. As one differentiates across the phenomena δ functions will appear at these locations. The flow is also not differentiable at the edges of the rarefaction wave although it is continuous there. Differentiation across the edges of that wave result in jump discontinuities in the sensitivities.

However, the flow solution can be differentiated within each of the five regions. The derivatives make sense as right or left limits of derivatives at the boundaries of the five regions.

The tangent linear model is obtained at the level code and it is the discrete equivalent of the linearization around the basic state. We computed the sensitivity of the flow variables (pressure, density and velocity) with respect to an initial parameter

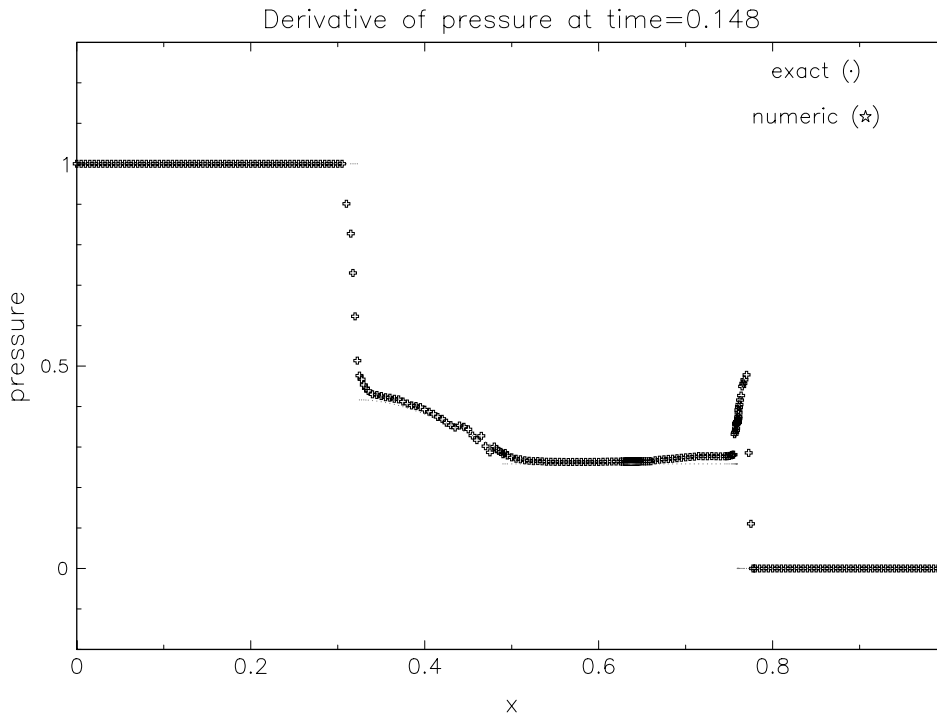


Fig. 2. Sensitivity with respect to the high initial pressure: numerical and exact values for pressure.

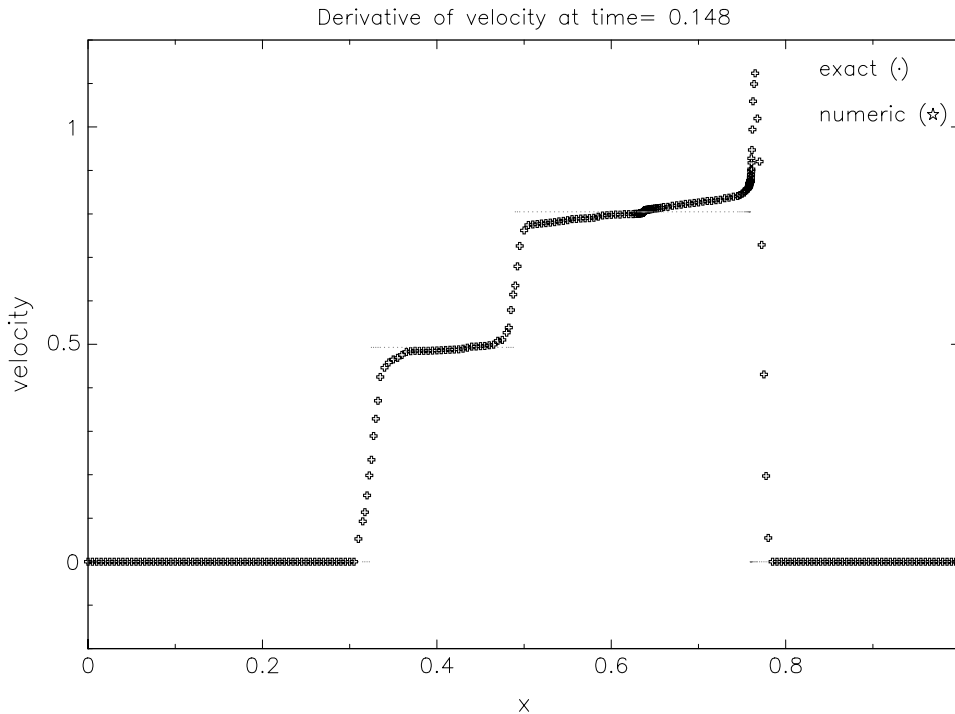


Fig. 3. Sensitivity with respect to the high initial pressure: numerical and exact values for velocity.

(the high pressure initial condition at the left of the membrane).

The numerical sensitivities show spikes at locations where the analytic derivatives do not exist. This is to be expected since the purpose of this research is to obtain numerical sensitivities which are *as close as possible* to the analytical sensitivities. Due to the sharp shock resolution of the original code the numerical spikes are an approximation to a Dirac measure at the points of discontinuities.

Our results (see Figs. 2–4) approximate very good the exact sensitivities in the five regions. We compare them with previously obtained numerical results (Gunzburger [10] computed the numerical sensitivity using finite differences, the sensitivity equation and automatic differentiation.) Our results show improvement both inside the five regions and at the edges of these regions where the flow is not differentiable and we think that this improvement is due to the use of adaptive mesh refinement in the forward code.

First we discuss our results at the locations where the flow is continuous (i.e., inside the five regions).

Both our plots and the graphs in [10] are practically the same as the analytical sensitivities on these regions. The only difference comes from the fact that in our case the numerical sensitivity is almost identical to the *exact* sensitivity over a larger proportion of the region than in [10].

At the edges of the five regions the situation is different. We have nondifferentiable points there which result in spikes in the graph of the analytical sensitivity and the numerical sensitivities attempt to approximate these spikes. The main difference between our results and the results in [10] can be seen around the location of the shock wave. The amplitude of the numerical spike in our case is 1.15 for the derivative of the velocity, 0.5 for the derivative of the pressure and 0.35 for the derivative of the density (compared to 3.5, 0.85 and 0.55 in [10]).

We chose the adaptive mesh refinement coupled with a Riemann solver as the forward code for the following reason: since the tangent linear model is obtained at code level from the original code we wanted to eliminate as much as possible the errors due to the

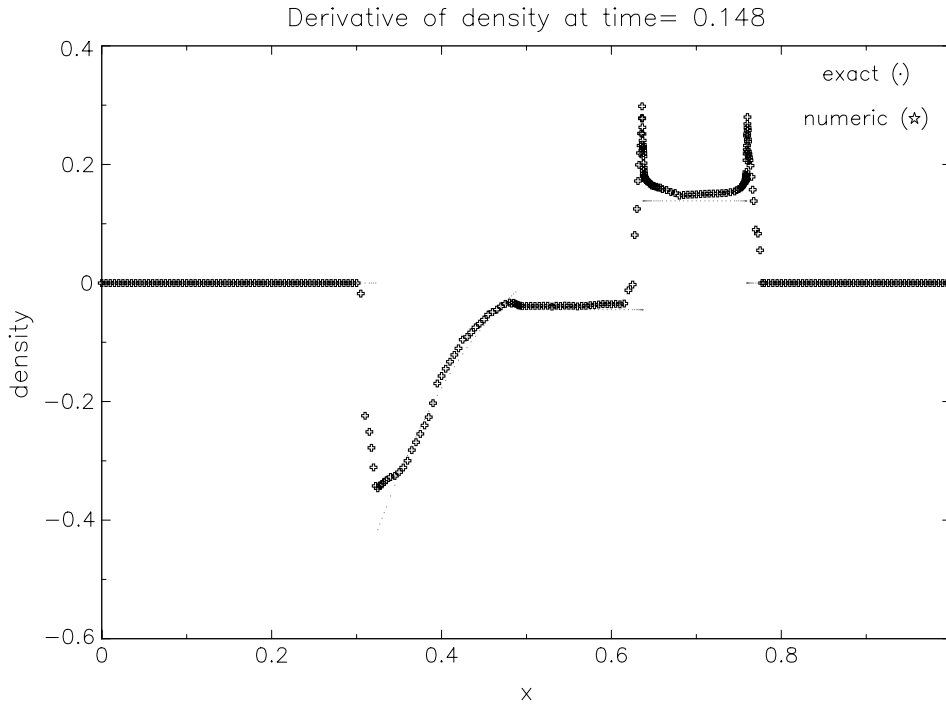


Fig. 4. Sensitivity with respect to the high initial pressure: numerical and exact values for density.

difference between the numerical flow and the analytical flow and we consider that for the code employed to solve the shock-tube problem the flow is extremely well solved.

Our experience with tangent linear models in higher dimensions (although the application did not involve nonsmooth functions [11]) suggests the possibility of application of the numerical methodology presented here for spatial higher dimensions. In the very near future we will apply it for problems in 2-D where we expect a decrease in the numerical accuracy of sensitivity computation. A possible remedy in order [5] to alleviate this problem is to apply a smoother to the sensitivities after they were computed using the tangent linear model.

7. Concluding remarks

Theoretical aspects of linearization for Euler equations were presented. The solution of the linearized system of equations and the sensitivity with respect to a model parameter satisfy the same tangent linear system. The tangent linear model provides a numerical

value of the sensitivity which is in better agreement with the analytical solution than any previously published numerical results, to a high extent due to the use of highly accurate adaptive mesh refinement code.

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Appendix A

Following a private communication from one of the reviewers we present the derivation of Eq. (12) using Eq. (1):

$$\begin{aligned} \frac{\partial \bar{\mathbf{V}}}{\partial t} + \frac{\partial}{\partial \hat{x}} \left(\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \bar{\mathbf{V}} \right) \\ = \frac{\partial \hat{\mathbf{V}}}{\partial t} - \frac{\partial \Psi}{\partial t} \frac{\partial \hat{\mathbf{U}}}{\partial \hat{x}} - \Psi \frac{\partial^2 \hat{\mathbf{U}}}{\partial t \partial \hat{x}} \end{aligned}$$

$$\begin{aligned}
& + \frac{\partial}{\partial \hat{x}} \left(\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \hat{\mathbf{V}} \right) \\
& - \frac{\partial}{\partial \hat{x}} \left(\left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \Psi \frac{\partial \hat{\mathbf{U}}}{\partial \hat{x}} \right) \\
& = - \frac{\partial}{\partial \hat{x}} \left(\Psi \left[\frac{\partial \hat{\mathbf{U}}}{\partial t} + \left(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t} \right) \frac{\partial \hat{\mathbf{U}}}{\partial \hat{x}} \right] \right) = 0.
\end{aligned}$$

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