Numerical and theoretical considerations for sensitivity calculation of discontinuous flow

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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 results.

Key words: sensitivity, Euler equations, discontinuity, linearization, sensitivity estimates, tangent linear model

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.

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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 (Burgreen and Baysal [1], Newman et al. [2], Taylor et al. [3], Mohammadi and Pironneau [4]), noise analysis and optimization of electronic circuits (Nguyen et al. [5]), control of contaminant releases in rivers (Piasecki and Katopodes [6]), control of water movement through sytems of irrigation canals (Sanders and Katopodes [7]), shallow water wave control (Sanders and Katopodes [8]), aeroelastic analysis (Giunta and Sobiesczanski-Sobieski [9]), shock sensitivity evaluations of dynamic financial strategies (Gourieroux and Jasiak [10])and meteorological applications (Navon et al. [11]).

Theoretical and computational aspects of sensitivity calculation in the presence of discontinuities were presented also by Ulbrich [12], Godlewski and Raviart [13], Bouchut and James [14] and DiCesare and Pironneau [15].

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:

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

where

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

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 $\varepsilon = \frac{P}{(\gamma-1)\rho}$ 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 2 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 Figure 1).

The exact solution can be found explicitly as a function of x and t (see Liepmann and Roshko [16]) and its plot (numerical solution versus analytical solution) is shown in Fig. 1. The solution has several distincts regions: a region of low pressure and density; an area between shock and contact discontinuity; an area between contact discontinuity and rarefaction wave; ararefaction 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

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

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

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

where $\frac{\partial N}{\partial \mathbf{X}}$ 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

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

To determine the sensitivity with respect to a parameter α we differentiate equation (3) and assuming that we can interchange the order of differentiation we obtain

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

which implies that the sensitivity $\dfrac{\partial \mathbf{X}}{\partial \alpha}$ with respect to the parameter α satisfies also the 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

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

$$\begin{aligned} \mathbf{U}^{\epsilon} &= \mathbf{U}(x,t) + \epsilon \mathbf{V}(x,t) \\ \mathbf{U}^{\epsilon} = \mathbf{U}(x,0) + \epsilon \mathbf{V}(x,0) &= \mathbf{U}_0(x) + \epsilon \mathbf{V}_0(x) \end{aligned}$$

with $\epsilon > 0$ a small parameter.

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

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

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

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

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 $\mathbf{U}^{\epsilon}$ presents a discontinuity along a different line $\mathbf{L}^{\epsilon} = \{(x,t), x = \Phi^{\epsilon}(t) = \Phi(t) + \epsilon\Psi(t), t \geq 0\}$ and at most weak discontinuities outside $\mathbf{L}^{\epsilon}$.

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 :

$$
\begin{aligned}
\hat{x} &= x - \Phi^\epsilon(t) && (7)\\
\hat{\mathbf{U}}^\epsilon(\hat{x},t) &= \mathbf{U}^\epsilon(\hat{x}+\Phi^\epsilon(t),t) && (8)
\end{aligned}
$$

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

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

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

$$
[F(\hat{\mathbf{U}}^\epsilon)] = \frac{\partial \Phi^\epsilon}{\partial t}[\hat{\mathbf{U}}^\epsilon] \qquad (10)
$$

Recalling that

$$
\begin{aligned}
\hat{\mathbf{U}}(\hat{x},t) &= \mathbf{U}(\hat{x}+\Phi(t),t)\\
\hat{\mathbf{U}}^\epsilon &= \hat{\mathbf{U}} + \epsilon\hat{\mathbf{U}} + \cdots\\
\Phi^\epsilon &= \Phi + \epsilon\Psi
\end{aligned}
$$

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

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

We define $\bar{\mathbf{V}}(\hat{x},t) = \hat{\mathbf{V}}(\hat{x},t) - \Psi(t)\dfrac{\partial \hat{\mathbf{U}}}{\partial \hat{x}}(\hat{x},t)$. Then the pair $(\bar{\mathbf{V}},\Psi)$ satisfies the equations and jump condition:

$$
\frac{\partial \bar{\mathbf{V}}^\epsilon}{\partial t} + \frac{\partial}{\partial \hat{x}}\Big(\Big(\mathbf{J}(\hat{\mathbf{U}}) - \frac{\partial \Phi}{\partial t}\Big)\bar{\mathbf{V}}) - \frac{\partial \Psi}{\partial t}\hat{\mathbf{U}}\Big) = 0 \qquad (12)
$$

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

The equations (12) have a unique solution (Godlewski [13]). The solution $\mathbf{V}$ of the system (6) is defined as the sum of a function and a measure whose support is $\mathbf{L}$

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

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 Majda [17] and Metivier [18]. 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

$$||u||^2_{L^2_\eta} = \int_\Omega e^{-2\eta t} |u(x)|^2 dx = ||e^{-\eta t} u||^2_{L^2}$$
$$||u||^2_{H^1_\eta} = ||e^{-\eta t} u||^2_{H^1} \tag{14}$$

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

$$\eta ||\bar{\mathbf{V}}||^2_0 + ||\bar{\mathbf{V}}|_{x=0}||^2_0 + ||\Psi||^2_{1,\eta} \le \frac{C}{\eta} ||e^{-\eta t}\mathbf{F}||^2_0 \tag{15}$$

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

6 Numerical considerations

To solve the Riemann problem we chose a code written by S. Li [19] which employs a method of Adaptive Mesh Refinement in conjunction with a Riemann solver of Roe-type (LeVeque [20]). 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.

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 (the high pressure initial condition at the left of the membrane). Our results (see Figure 2) show a marked improvement over previous numerical results (Gunzburger [21]). This improvement can be especially seen in regions where discontinuities are present and it can be characterized by a smaller size of the "spikes" appearing due to nondifferentiability.

Among the reasons which contributed to the "better" accuracy of the sensitivity one may enumerate the adaptive mesh refinement and the employment of a special error estimator for the tangent linear code (in addition to the error estimator implemented in the original code).

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 results.

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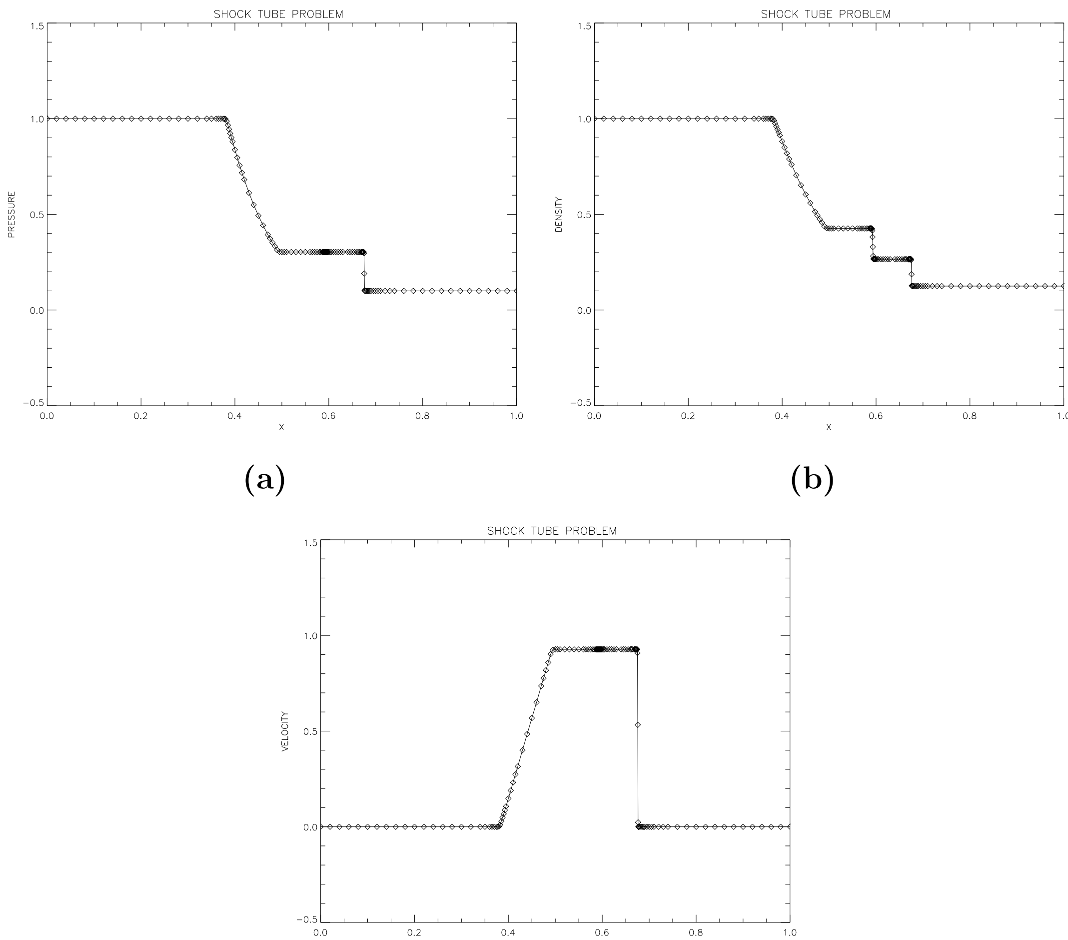
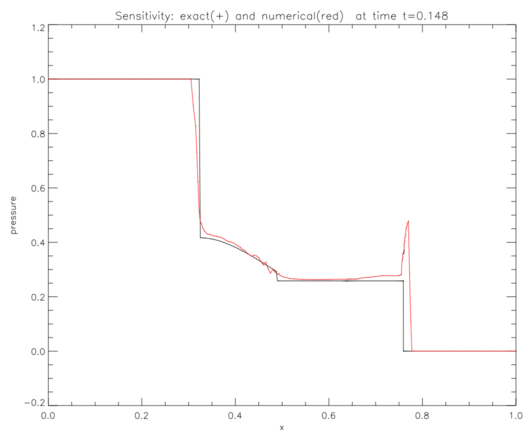


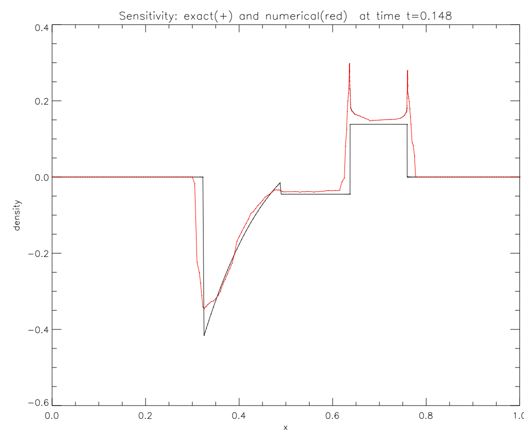
(a) **(b)**

(c)

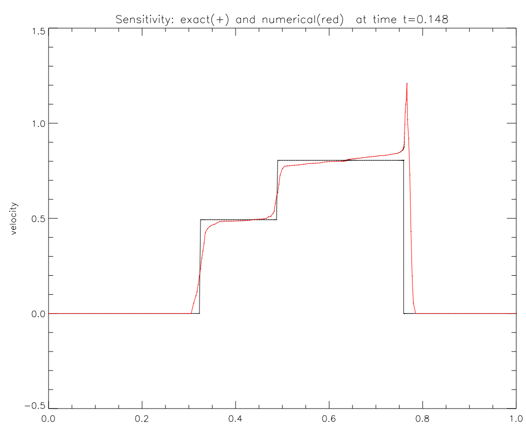
Fig. 1. Exact solution of the shock-tube problem: numerical (◇) and analytical (—) for a) pressure, b) density and c) velocity.



(a)



(b)



(c)

Fig. 2. Sensitivity with respect to the high initial pressure: numerical (red line) and analytical (—) for a) pressure, b) density and c) velocity.