Chapter 10

Sensitivity Equations for Hyperbolic Systems

10.1. Introduction

Most conservation laws presented in the previous chapters involve flux functions or source terms that are functions of the conserved variable U and a number of parameters that are known *a priori*. For instance, the flux F in linear advection equations (section 1.3) is equal to the product of the conserved variable AC by the flow velocity u. The knowledge of u is required to solve the equation. In the kinematic wave equations (section 1.5), the friction coefficient, channel slope and channel geometry are parameters on which the discharge Q depends. In the Buckley-Leverett equation (section 1.6), the flux F is a function of the conserved variable s, the shape parameter b_{BL} and the Darcy velocity V_d. In the advection-adsorption equation (section 1.7), the parameters are the flow velocity and the adsorption constants (k_{lin} for a linear law, k_{F} and b in a Freundlich model, k_{L} and C_{L} in a Langmuir-based model). The initial conditions may also be considered as a parameter in the problem that consists of solving the equations over time.

In practical engineering applications, the parameters are known with a given imprecision or uncertainty. It is sometimes impossible to measure these parameters directly, hence the need for a "calibration" of the model. Calibration consists of adjusting or constraining the parameters so that the model output reproduces measurements or observations as faithfully as possible. In some other cases, such as scenario analysis, the modeler is interested in knowing the consequences of imprecision or uncertainty in the knowledge of the parameters on the model output.

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In optimization and control problems, we are interested in the parameter values that allow a certain objective (or cost) function to be minimized.

In all these problems, the sensitivity of the solution to the model parameters (that is, how the output variables change with the parameters) plays an essential role. For instance, trying to "calibrate" a model parameter to which the model output is not sensitive would be meaningless. In contrast, oversensitivity of a model to a given parameter may indicate the hidden influence of additional parameters that have not been identified. Model sensitivity is used in optimization problems for optimum search. In uncertainty analysis, it can be used in the framework of efficient, first-order second moment techniques. In the field of flow control, it is often used in the framework of adjoint modeling.

Sensitivity is classically defined as the partial derivative of a model variable with respect to a parameter. Cacuci [CAC 03] defines the sensitivity as a Gateaux (also called directional) derivative. Several techniques may be used to compute the sensitivity of a model variable to a parameter:

– The empirical, or finite difference approach, consists of carrying out a simulation using two slightly different values of the parameter of interest. The sensitivity is defined as the limit of the ratio of the variation in the variable to the variation in the parameter. This approach is very efficient in estimating the sensitivity of a model, the governing equations of which are unknown. It may also be used in the local sensitivity analysis of models with known governing equations, such as hyperbolic systems of conservation laws.

– The complex differentiation technique [LYN 67] consists of introducing a pure imaginary perturbation in the parameter of interest (see [LU 07] for an application). The solution of the governing equations is a complex number, the imaginary part of which is used to compute the sensitivity. This technique is second-order accurate with respect to the perturbation in the parameter. It has the advantage that only one run of the model is needed. The drawback is that all the mathematical operations in the model must be carried out on complex numbers, which is computationally expensive.

– Code differentiation consists of differentiating the programmed instructions instead of the governing equations in the informatic implementation of the model. Code differentiation may be manual or automatic [ELI 07].

– Analytical differentiation consists of differentiating the analytical solution of the governing equations with respect to the parameter. This implies that (i) an analytical solution is available, which is not often the case in real-world problems, and (ii) the parameter is assumed to be perturbed uniformly over the entire solution domain. This is another constraining assumption.

– Direct sensitivity calculation consists of differentiating the governing equations of the model with respect to the parameter of interest, thus yielding a set of governing sensitivity equations. The sensitivity equations are solved in a coupled way with the original model equations. This approach is examined in the present chapter. Two types of sensitivity equations are considered hereafter: forward (or direct) sensitivity equations, and adjoint (or backward) sensitivity equations.

A particular aspect of sensitivity equations for hyperbolic systems is that the solutions of the hyperbolic system may become locally discontinuous. In this case, the derivatives of the solution with respect to time, space and the parameter of interest become locally undefined and the sensitivity equations must be modified because sensitivity becomes a locally non-conserved variable (see section 10.2.2). Classical numerical techniques yield unstable sensitivity solutions [GUN 99]. The governing sensitivity equations must be modified to account for this (see [BAR 02], where the governing sensitivity equations are reformulated in the framework of the theory of distributions).

10.2. Forward sensitivity equations for scalar laws

10.2.1. *Derivation for continuous solutions*

Consider a one-dimensional scalar hyperbolic equation written in the conservation form [1.1], recalled here:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = S$$

where U, F and S are respectively the conserved variable, the flux and the source term. In what follows, F and S are functions in the form:

$$\left.\begin{aligned} F &= F(U, \varphi) \\ S &= S(U, \varphi) \end{aligned}\right\} \qquad [10.1]$$

where φ is a parameter with respect to which the sensitivity analysis is to be carried out. φ may be a parameter in the conservation law, in the initial or boundary conditions.

The purpose is to study the influence of variations in φ on the solution U over the solution domain. This is done via a perturbation analysis. The parameter φ is expressed in the form:

$$\varphi(x,t) = \varphi_0(x,t) + \varepsilon(x,t)\varphi' \qquad [10.2]$$

where φ_0 and φ' are respectively the "nominal" value of the parameter and φ' is an infinitesimal perturbation. $\varepsilon(x, t)$ is called the support, or characteristic function of the perturbation. It expresses the fact that the parameter may not be perturbed with the same magnitude at all points and all times of the solution domain. The solution of equation [1.1] with F, S and φ as defined in equations [10.1–2] is written in the form:

$$U(x,t) = U_0(x,t) + U'(x,t) \qquad [10.3]$$

where U_0 is the solution of equation [1.1] for $\varphi = \varphi_0$ and U' is the perturbation in U caused by the perturbation in φ. The sensitivity of U with respect to φ is defined as the limit:

$$s(x,t) = \lim_{\varphi' \to 0} \frac{U'(x,t)}{\varphi'} \qquad [10.4]$$

The governing equation for s is obtained by writing two equations [1.1] with two different values of φ':

$$\left.\begin{aligned} \frac{\partial U_0}{\partial t} + \frac{\partial}{\partial x} F(U_0, \varphi_0) &= S(U_0, \varphi_0) \\ \frac{\partial}{\partial t}(U_0 + U') + \frac{\partial}{\partial x} F(U_0 + U', \varphi_0 + \varepsilon\varphi') &= S(U_0 + U', \varphi_0 + \varepsilon\varphi') \end{aligned}\right\} \qquad [10.5]$$

A first-order Taylor series expansion yields:

$$\left.\begin{aligned} F(U_0 + U', \varphi_0 + \varepsilon\varphi') &\approx F(U_0, \varphi_0) + \frac{\partial F}{\partial U} U' + \frac{\partial F}{\partial \phi} \varepsilon\varphi' \\ S(U_0 + U', \varphi_0 + \varepsilon\varphi') &\approx S(U_0, \varphi) + \frac{\partial S}{\partial U} U' + \frac{\partial S}{\partial \phi} \varepsilon\varphi' \end{aligned}\right\} \qquad [10.6]$$

Substituting equations [10.6] into equations [10.5] and subtracting yields:

$$\frac{\partial U'}{\partial t} + \frac{\partial}{\partial x}\left[\frac{\partial F}{\partial U} U' + \frac{\partial F}{\partial \varphi} \varepsilon\varphi'\right] = \frac{\partial S}{\partial U} U' + \frac{\partial S}{\partial \varphi} \varepsilon\varphi' \qquad [10.7]$$

Dividing equation [10.7] by the perturbation φ' and introducing definition [10.4] gives:

$$\frac{\partial s}{\partial t}+\frac{\partial}{\partial x}\left[\frac{\partial F}{\partial U}s+\frac{\partial F}{\partial \varphi}\varepsilon\right]=\frac{\partial S}{\partial U}s+\varepsilon\frac{\partial S}{\partial \varphi} \qquad [10.8]$$

Noting from Chapter 1 that $\partial F/\partial U$ is defined as the wave speed λ, equation [10.8] becomes:

$$\frac{\partial s}{\partial t}+\frac{\partial G}{\partial x}=\frac{\partial S}{\partial U}s+\varepsilon\frac{\partial S}{\partial \varphi}-\frac{\partial}{\partial x}\left(\varepsilon\frac{\partial F}{\partial \varphi}\right), \qquad G=\lambda s \qquad [10.9]$$

10.2.2. *Conservation, non-conservation and characteristic forms*

Equations [1.1] and [10.9] can be written in vector conservation form as:

$$\frac{\partial \mathrm{V}}{\partial t}+\frac{\partial \mathrm{H}}{\partial x}=\mathrm{T} \qquad [10.10]$$

where V, H and T are defined as:

$$\begin{aligned}&\mathrm{V}=\begin{bmatrix}U\\ s\end{bmatrix}, \qquad \mathrm{H}=\begin{bmatrix}F\\ G\end{bmatrix}=\begin{bmatrix}F\\ \lambda s\end{bmatrix},\\ &\mathrm{T}=\begin{bmatrix}S\\ Q\end{bmatrix}=\begin{bmatrix}S\\ \dfrac{\partial S}{\partial U}s+\varepsilon\dfrac{\partial S}{\partial \varphi}-\dfrac{\partial}{\partial x}\left(\varepsilon\dfrac{\partial F}{\partial \varphi}\right)\end{bmatrix}\end{aligned} \qquad [10.11]$$

The non-conservation form of [10.10] is obtained by differentiating H with respect to V:

$$\frac{\partial \mathrm{V}}{\partial t}+\mathrm{B}\frac{\partial \mathrm{V}}{\partial x}=\mathrm{T}' \qquad [10.12]$$

with:

$$\mathrm{B}=\begin{bmatrix}\lambda & 0\\ \lambda_U s & \lambda\end{bmatrix}, \qquad \mathrm{T}'=\mathrm{T}-\left(\frac{\partial \mathrm{H}}{\partial x}\right)_{\mathrm{V=Const}} \qquad [10.13]$$

where λ_U is the derivative of λ with respect to U. The matrix B has a double eigenvalue, $\lambda^{(1)}=\lambda^{(2)}=\lambda$. System [10.12] is not strictly hyperbolic because a necessary condition for hyperbolicity is that all the eigenvalues of the Jacobian matrix be distinct. System [10.10–11] is said to be linearly degenerate.

The characteristic form of sensitivity equations is derived directly from equations [1.17] and [10.12]:

$$\left.\begin{aligned} &\frac{\partial U}{\partial t}+\lambda\frac{\partial U}{\partial x}=S-\left(\frac{\partial F}{\partial x}\right)_{U=\text{Const}} \\ &\frac{\partial s}{\partial t}+\lambda\frac{\partial s}{\partial x}=\frac{\partial S}{\partial U}s+\varepsilon\frac{\partial S}{\partial \varphi}-\frac{\partial}{\partial x}\left(\varepsilon\frac{\partial F}{\partial \varphi}\right)-\frac{\partial \lambda}{\partial x}s-\left(\frac{\partial G}{\partial x}\right)_{\substack{U=\text{Const}\\ s=\text{Const}}} \end{aligned}\right\} \qquad [10.14]$$

This system can be written in vector form as:

$$\frac{\mathrm{dV}}{\mathrm{d}t}=\text{T" for}\frac{\mathrm{d}x}{\mathrm{d}t}=\lambda \qquad [10.15]$$

Both the conserved variable U and its sensitivity s are Riemann invariants for system [10.10]. In the absence of source term Q", U and s are constant along the characteristics.

10.2.3. *Extension to discontinuous solutions*

Chapter 3 deals with the properties of discontinuous solutions U for the original hyperbolic conservation law [1.1] (see section 3.4). Discontinuous solutions verify the jump relationship [3.28], recalled here:

$$(U_1-U_2)c_s=F_1-F_2$$

where subscripts 1 and 2 denote the values of U on the left- and right-hand sides of the discontinuity, and c_s is the speed of the discontinuity. This relationship cannot be transposed as such to the sensitivity. As shown in [BAR 02], extra terms appear in the jump relationship for the sensitivity equations. Several derivation methods are available for the sensitivity jump relationships:

– A first approach consists of carrying out two balances over an infinitesimal control volume $[x_1, x_2]$ containing the discontinuity. The first is written for the "nominal" value φ_0 of the parameter, the second is carried out for the perturbed value $\varphi_0 + \varepsilon\varphi'$. This approach is presented in [GUI 09c] and will not be detailed here.

– Another possible approach consists of representing the propagation of the discontinuity in the (x, φ) plane for a given time t and linking both sides of the discontinuity using two different paths (Figure 10.1). This approach is used hereafter.

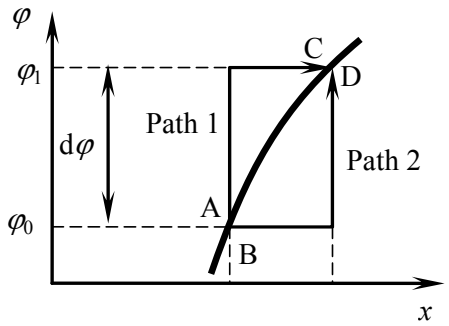

Figure 10.1. *Representation of a discontinuity in the (x,φ) plane for a given time t*

The jump relationships are written for two different values of the parameter: the nominal value φ_0 and a slightly different value $\varphi_1 = \varphi_0 + \mathrm{d}\varphi$. The points on the left- and right-hand sides of the discontinuity for $\varphi = \varphi_0$ are denoted by A and B respectively. The points on the left- and right-hand sides of the discontinuity for $\varphi = \varphi_1$ are denoted by C and D respectively. The jump relationships hold:

$$\left.\begin{aligned} F_{\mathrm{A}} - F_{\mathrm{B}} &= (U_{\mathrm{A}} - U_{\mathrm{B}})\, c_s(\varphi_0) \\ F_{\mathrm{C}} - F_{\mathrm{D}} &= (U_{\mathrm{C}} - U_{\mathrm{D}})\, c_s(\varphi_1) \end{aligned}\right\} \qquad [10.16]$$

Connecting the points A and C along Path 1 and points B and D along Path 2 yields:

$$\left.\begin{aligned} F_{\mathrm{C}} - F_{\mathrm{A}} &= (x_{\mathrm{C}} - x_{\mathrm{A}})\frac{\partial F}{\partial x} + (\varphi_1 - \varphi_0)\frac{\partial F}{\partial \varphi} = \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial F}{\partial x}\right)_{\mathrm{L}} + G_{\mathrm{L}}\right]\mathrm{d}\varphi \\ F_{\mathrm{D}} - F_{\mathrm{B}} &= \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial F}{\partial x}\right)_{\mathrm{R}} + G_{\mathrm{R}}\right]\mathrm{d}\varphi \\ U_{\mathrm{C}} - U_{\mathrm{A}} &= \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial U}{\partial x}\right)_{\mathrm{L}} + \left(\frac{\partial U}{\partial \varphi}\right)_{\mathrm{L}}\right]\mathrm{d}\varphi = \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial U}{\partial x}\right)_{\mathrm{L}} + s_{\mathrm{L}}\right]\mathrm{d}\varphi \\ U_{\mathrm{D}} - U_{\mathrm{B}} &= \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial U}{\partial x}\right)_{\mathrm{R}} + \left(\frac{\partial U}{\partial \varphi}\right)_{\mathrm{R}}\right]\mathrm{d}\varphi = \left[\frac{\partial x_s}{\partial \varphi}\left(\frac{\partial U}{\partial x}\right)_{\mathrm{R}} + s_{\mathrm{R}}\right]\mathrm{d}\varphi \end{aligned}\right\} \qquad [10.17]$$

where x_s is the abscissa of the shock. Subtracting equations [10.16] from one another leads to:

$$\begin{aligned} F_{\mathrm{C}} - F_{\mathrm{A}} - (F_{\mathrm{D}} - F_{\mathrm{B}}) &= (U_{\mathrm{C}} - U_{\mathrm{D}})\, c_s(\varphi_1) - (U_{\mathrm{A}} - U_{\mathrm{B}})\, c_s(\varphi_0) \\ &= [(U_{\mathrm{C}} - U_{\mathrm{A}}) - (U_{\mathrm{D}} - U_{\mathrm{B}})]\, c_s(\varphi_0) \\ &\quad + (U_{\mathrm{C}} - U_{\mathrm{D}}) \frac{\partial c_s}{\partial \varphi} \mathrm{d}\varphi \end{aligned} \qquad [10.18]$$

Substituting relationships [10.17] into [10.18] and simplifying by $\mathrm{d}\varphi$ leads to:

$$\left.\begin{aligned} &(s_{\mathrm{L}} - s_{\mathrm{R}})c_s = G_{\mathrm{L}} - G_{\mathrm{R}} + R \\ &R = \left[\left(\frac{\partial F}{\partial x} - c_s \frac{\partial U}{\partial x}\right)_{\mathrm{L}} - \left(\frac{\partial F}{\partial x} - c_s \frac{\partial U}{\partial x}\right)_{\mathrm{R}}\right] \frac{\partial x_s}{\partial \varphi} - (U_{\mathrm{L}} - U_{\mathrm{R}}) \frac{\partial c_s}{\partial \varphi} \end{aligned}\right\} \qquad [10.19]$$

where subscripts L and R denote the values on the left- and right-hand sides of the discontinuity. Compared to the original Rankin-Hugoniot condition [3.28], the first equation [10.19] contains an extra source term R that takes effect only at discontinuities. The expression of the source term Q in equation [10.11] is modified into:

$$\mathrm{T} = \left[\frac{\partial S}{\partial U} s + \varepsilon \frac{\partial S}{\partial \varphi} - \frac{S}{\partial x}\left(\varepsilon \frac{\partial F}{\partial \varphi}\right) + R\, \delta_{x_s} \right] \qquad [10.20]$$

where δ_{x_s} is Dirac's function centered at $x = x_s$ and R is the extra source term as defined in [10.19].

10.2.4. *Solution of the Riemann problem*

10.2.4.1. *Definition*

The Riemann problem is defined for the hyperbolic part (that is, without source term) of equation [10.10]:

$$\left.\begin{aligned} &\frac{\partial \mathrm{V}}{\partial t} + \frac{\partial \mathrm{H}}{\partial x} = 0 \\ &\mathrm{V}(x,0) = \begin{cases} \mathrm{V_L} & \text{for } x < x_0 \\ \mathrm{V_R} & \text{for } x < x_0 \end{cases} \end{aligned}\right\} \qquad [10.21]$$

The properties of the solution of the Riemann problem are detailed in Chapter 4. The properties of the solutions of the Riemann problem for the sensitivity equations of scalar hyperbolic conservation laws are given in [GUI 07]. The reader is referred to the original publication for the details of the proofs, only the broad lines being recalled hereafter.

Recall from Chapter 4 that the solution of the Riemann problem for a convex or concave scalar hyperbolic law is made of a simple wave connecting the left and right states of the Riemann problem. If the flux function is non-convex, the wave may be a compound wave, that is, the combination of a rarefaction wave and a shock. The solution of the Riemann problem is self-similar regardless of the nature of the wave. In other words, the solution U is a function of the ratio $(x - x_0)/t$ alone.

10.2.4.2. *Solution for a convex or concave law*

The following configurations are considered for a convex or concave law.

(1) Rarefaction wave (Figure 10.2a). This is the case if $\lambda_L = \lambda(U_L) < \lambda_R = \lambda(U_R)$. Then the solution U is given by:

$$U(x,t) = \begin{cases} U_L & \text{for } x \le x_0 + \lambda_L t \\ \lambda^{-1}\left[(x - x_0)/t\right] & \text{for } x_0 + \lambda_L t \le x \le x_0 + \lambda_R t \\ U_R & \text{for } x \ge x_0 + \lambda_R t \end{cases} \quad [10.22]$$

where the function $\lambda^{-1}(\xi)$ is the inverse function of $\lambda(U)$. The rarefaction wave can be shown to be a void sensitivity region [GUI 07], that is, the sensitivity is zero within a rarefaction wave:

$$s(x,t) = \begin{cases} s_L & \text{for } x < x_0 + \lambda_L t \\ 0 & \text{for } x_0 + \lambda_L t < x < x_0 + \lambda_R t \\ s_R & \text{for } x > x_0 + \lambda_R t \end{cases} \quad [10.23]$$

(2) Contact discontinuity (Figure 10.2b). This type of wave verifies $\lambda_L = \lambda_R = \lambda_{LR}$. In such a case, the solution U of the Riemann problem is:

$$U(x,t) = \begin{cases} U_L & \text{for } x < x_0 + \lambda_{LR} t \\ U_R & \text{for } x > x_0 + \lambda_{LR} t \end{cases} \quad [10.24]$$

The sensitivity s is given by:

$$s(x,t) = \begin{cases} s_L & \text{for } x < x_0 + \lambda_{LR} t \\ s_R & \text{for } x > x_0 + \lambda_{LR} t \end{cases} \quad [10.25]$$

Note that $\lambda_L = \lambda_R$ by definition of the contact discontinuity. This is not necessarily an indication that $R = 0$ in equation [10.19], because $\partial\lambda / \partial\varphi$ (to mention but one of the terms in [10.19]) may be non-zero.

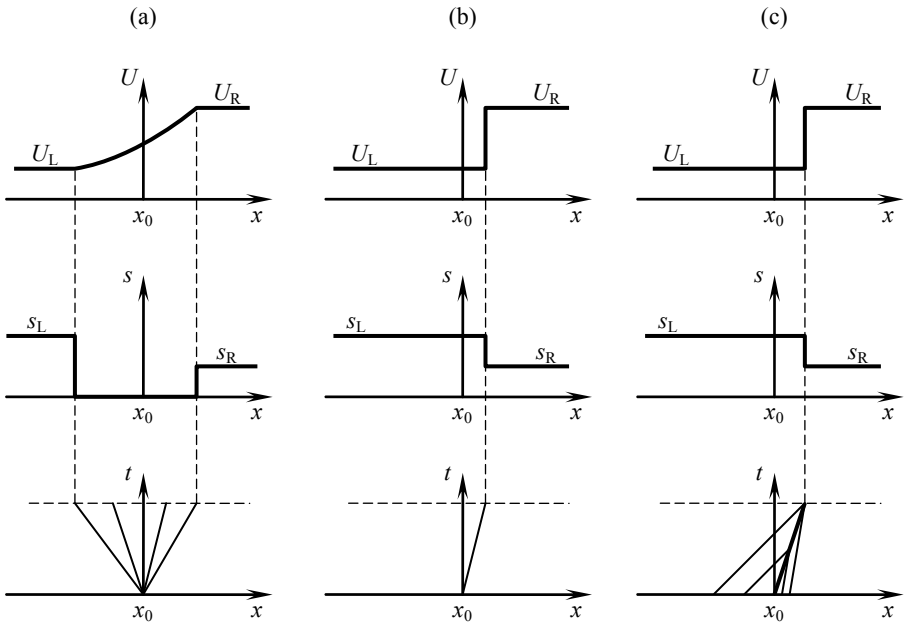

Figure 10.2. *Solution of the Riemann problem for a convex/concave law. (a) rarefaction wave; (b) contact discontinuity; (c) shock wave*

(3) Shock wave (Figure 10.2c). For a convex law, this is the case if $\lambda_L > \lambda_R$. U is given by:

$$U(x,t) = \begin{cases} U_L & \text{for } x < x_0 + c_s t \\ U_R & \text{for } x > x_0 + c_s t \end{cases} \qquad [10.26]$$

The sensitivity is discontinuous across the shock. Since s is a Riemann invariant, it verifies:

$$s(x,t) = \begin{cases} s_L & \text{for } x < x_0 + c_s t \\ s_R & \text{for } x > x_0 + c_s t \end{cases} \qquad [10.27]$$

10.2.4.3. *Non-convex conservation laws*

In addition to the three configurations presented in section 10.2.4.2 non-convex flux functions give rise to a fourth possible configuration.

(4) Compound (mixed) wave: a rarefaction wave bounded by a shock. This configuration appears when the left and right state of the Riemann problem located on both sides of the value $U_{\max}$ for which the wave speed λ is maximum (see Chapter 4):

$$\left.\begin{array}{l} U_{\mathrm{L}} < U_{\max} < U_{\mathrm{R}} \\ U_{\mathrm{R}} < U_{\max} < U_{\mathrm{L}} \\ \dfrac{\mathrm{d}\lambda}{\mathrm{d}U}(U_{\max}) = 0 \end{array}\right\} \qquad [10.28]$$

Then U is given by:

$$U(x,t) = \begin{cases} U_{\mathrm{L}} & \text{for } x \le x_0 + \lambda_{\mathrm{L}} t \\ \lambda^{-1}\left[(x - x_0)/t\right] & \text{for } x_0 + \lambda_{\mathrm{L}} t \le x < x_0 + \lambda_{\mathrm{R}} t \\ U_{\mathrm{R}} & \text{for } x > x_0 + \lambda_{\mathrm{R}} t \end{cases} \qquad [10.29]$$

for a mixed wave with a shock facing to the right (Figure 10.3a), and by:

$$U(x,t) = \begin{cases} U_{\mathrm{L}} & \text{for } x < x_0 + \lambda_{\mathrm{L}} t \\ \lambda^{-1}\left[(x - x_0)/t\right] & \text{for } x_0 + \lambda_{\mathrm{L}} t < x \le x_0 + \lambda_{\mathrm{R}} t \\ U_{\mathrm{R}} & \text{for } x \ge x_0 + \lambda_{\mathrm{R}} t \end{cases} \qquad [10.30]$$

for a mixed wave with a shock facing to the left (Figure 10.3b).

In both cases the sensitivity is zero within the rarefaction wave. It verifies equation [10.22].

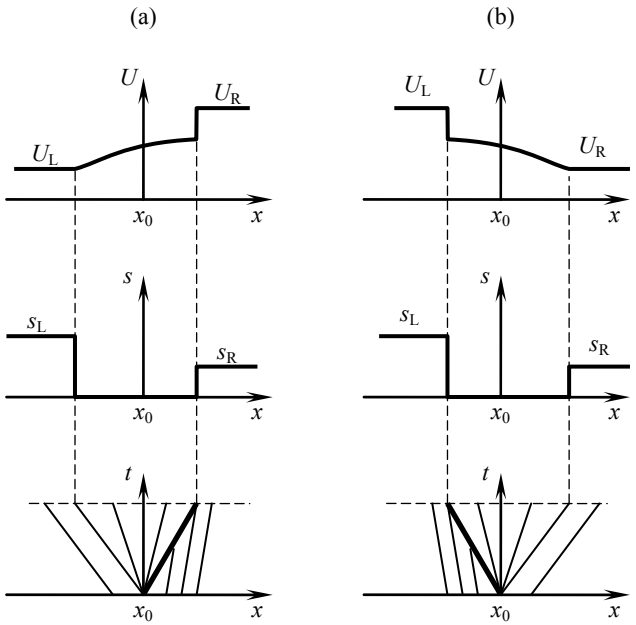

Figure 10.3. *Solution of the Riemann problem for a non-convex law: compound (mixed) wave: (a) shock on the right-hand side of the wave; (b) shock on the left-hand side of the wave*

10.3. Forward sensitivity equations for hyperbolic systems

10.3.1. *Governing equations*

The governing sensitivity equations for hyperbolic systems are derived as explained in section 10.2. Consider the conservation form [2.2] of a hyperbolic system:

$$\frac{\partial \mathrm{U}}{\partial t} + \frac{\partial \mathrm{F}}{\partial x} = \mathrm{S}$$

where F and S are functions of the conserved variable U and the parameter φ:

$$\left.\begin{aligned} \mathrm{F} &= \mathrm{F}(\mathrm{U}, \varphi) \\ \mathrm{S} &= \mathrm{S}(\mathrm{U}, \varphi) \end{aligned}\right\} \qquad [10.31]$$

As in section 10.2, the parameter φ is subjected to an infinitesimal perturbation (equation [10.2]). Since both the "nominal" solution U and the perturbed solution U + U' verify equation [2.2], we have:

$$\left.\begin{aligned} \frac{\partial \mathrm{U}}{\partial t} + \frac{\partial}{\partial x}\mathrm{F}(\mathrm{U},\varphi) &= \mathrm{S}(\mathrm{U},\varphi) \\ \frac{\partial}{\partial t}(\mathrm{U}+\mathrm{U}') + \frac{\partial}{\partial x}\mathrm{F}(\mathrm{U}+\mathrm{U}',\varphi+\varepsilon\varphi') &= \mathrm{S}(\mathrm{U}+\mathrm{U}',\varphi+\varepsilon\varphi') \end{aligned}\right\} \qquad [10.32]$$

Subtracting equations [10.32] from each other, dividing by φ' and using the definition of the sensitivity vector $\mathrm{s} = \partial \mathrm{F}/\partial\varphi = \mathrm{U}'/\varphi'$ leads to the following sensitivity equations (see [GUI 09c] for the details of the derivation):

$$\left.\begin{aligned} &\frac{\partial \mathrm{s}}{\partial t} + \frac{\partial \mathrm{G}}{\partial x} = \mathrm{Q} \\ &\mathrm{G} = \mathrm{A}\mathrm{s} \\ &\mathrm{Q} = \frac{\partial \mathrm{S}}{\partial \mathrm{U}}\mathrm{s} + \varepsilon\frac{\partial \mathrm{S}}{\partial\varphi} - \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial \mathrm{F}}{\partial\varphi}\right) + \mathrm{R}\,\delta_s \\ &\mathrm{R} = \left[\left(\frac{\partial \mathrm{F}}{\partial x} - c_s\frac{\partial \mathrm{U}}{\partial x}\right)_{\mathrm{L}} - \left(\frac{\partial \mathrm{F}}{\partial x} - c_s\frac{\partial \mathrm{U}}{\partial x}\right)_{\mathrm{R}}\right]\frac{\partial x_s}{\partial\varphi} - (\mathrm{U}_{\mathrm{L}} - \mathrm{U}_{\mathrm{R}})\frac{\partial c_s}{\partial\varphi} \end{aligned}\right\} \qquad [10.33]$$

where $\mathrm{A} = \partial \mathrm{F}/\partial \mathrm{U}$ and δ_s is Dirac's function that takes effect only at shocks. The subscripts L and R in the definition of the point source term R indicate the values of the variables on the left- and right-hand side of the shock respectively. Equation [10.33] is valid for both continuous and discontinuous solutions. Note that the jump relationships for the sensitivity are obtained as the vector version of equations [10.19]:

$$\left.\begin{aligned} &(\mathrm{s}_{\mathrm{L}} - \mathrm{s}_{\mathrm{R}})\mathrm{c}_s = \mathrm{G}_{\mathrm{L}} - \mathrm{G}_{\mathrm{R}} + \mathrm{R} \\ &\mathrm{R} = \left[\left(\frac{\partial \mathrm{F}}{\partial x} - c_s\frac{\partial \mathrm{U}}{\partial x}\right)_{\mathrm{L}} - \left(\frac{\partial \mathrm{F}}{\partial x} - c_s\frac{\partial \mathrm{U}}{\partial x}\right)_{\mathrm{R}}\right]\frac{\partial x_s}{\partial\varphi} - (\mathrm{U}_{\mathrm{L}} - \mathrm{U}_{\mathrm{R}})\frac{\partial c_s}{\partial\varphi} \end{aligned}\right\} \qquad [10.34]$$

Equations [2.2] and [10.33] are rewritten in the form of a single system defining a variable V as the union of U and s:

$$\frac{\partial \mathrm{V}}{\partial t} + \frac{\partial \mathrm{H}}{\partial x} = \mathrm{T} \qquad [10.35]$$

where V, H and T are defined as:

$$\begin{aligned} \mathrm{V} &= \left[U_1, \ldots, U_m, s_1 \ldots, U_m\right]^T \\ \mathrm{H} &= \left[F_1, \ldots, F_m, G_1 \ldots, G_m\right]^T \\ T &= \left[S_1, \ldots, S_m, Q_1 \ldots, Q_m\right]^T \end{aligned} \qquad [10.36]$$

10.3.2. *Non-conservation and characteristic forms*

The non-conservation form [10.12] is recalled:

$$\frac{\partial \mathrm{V}}{\partial t} + \mathrm{B}\frac{\partial \mathrm{V}}{\partial x} = \mathrm{T}'$$

where T' is defined as in equation [10.13] by the union of two vectors:

$$\mathrm{T}' = \mathrm{T} - \left(\frac{\partial \mathrm{H}}{\partial x}\right)_{\mathrm{V=Const}} = \begin{bmatrix} \mathrm{S}' \\ \mathrm{Q}' \end{bmatrix} = \begin{bmatrix} \mathrm{S} - (\partial \mathrm{F}/\partial x)_{\mathrm{U=Const}} \\ \mathrm{Q} - (\partial \mathrm{G}/\partial x)_{\substack{\mathrm{U=Const} \\ \mathrm{s=Const}}} \end{bmatrix} \qquad [10.37]$$

and B is the square matrix defined as the union of four square matrices:

$$\mathrm{B} = \begin{bmatrix} \mathrm{A} & 0 \\ \mathrm{C} & \mathrm{A} \end{bmatrix} \qquad [10.38]$$

where A and C are the square Jacobian matrices:

$$\left.\begin{aligned} \mathrm{A} &= \frac{\partial \mathrm{F}}{\partial \mathrm{U}} = \frac{\partial \mathrm{G}}{\partial \mathrm{s}} \\ \mathrm{C} &= \frac{\partial \mathrm{G}}{\partial \mathrm{U}} \end{aligned}\right\} \qquad [10.39]$$

The first row in matrix B is related to the non-conservation form for the variable U, the second row expresses the non-conservation form for the sensitivity s. Note that $\partial \mathrm{G}/\partial \mathrm{s} = \mathrm{A}$ because $\mathrm{G} = \mathrm{As}$. A particular consequence is that all the eigenvalues of system [10.35] with B defined as in equation [10.38] are double because an eigenvalue for the conserved variable U is also an eigenvalue for the sensitivity s. The system is said to be linearly degenerate.

The characteristic form for U is derived in Chapter 2 and will not be recalled here. The characteristic form for s is obtained as follows. The vector equation [10.12] is written for the sensitivity only:

$$\frac{\partial \mathrm{s}}{\partial t} + \mathrm{A}\frac{\partial \mathrm{s}}{\partial x} = -\mathrm{C}\frac{\partial \mathrm{U}}{\partial x} + \mathrm{Q}' \qquad [10.40]$$

and the system is diagonalized by left-multiplying equation [10.40] with the inverse of the matrix K of eigenvectors of A:

$$\mathrm{K}^{-1}\frac{\partial \mathrm{s}}{\partial t} + \mathrm{K}^{-1}\mathrm{A}\mathrm{K}\,\mathrm{K}^{-1}\frac{\partial \mathrm{s}}{\partial x} = \mathrm{K}^{-1}\left(\mathrm{Q}' - \mathrm{C}\frac{\partial \mathrm{U}}{\partial x}\right) \qquad [10.41]$$

Introducing the diagonal matrix Λ formed by the eigenvalues of A, equation [10.41] is rewritten as:

$$\mathrm{K}^{-1}\frac{\partial \mathrm{s}}{\partial t} + \Lambda\,\mathrm{K}^{-1}\frac{\partial \mathrm{s}}{\partial x} = \mathrm{K}^{-1}\left(\mathrm{Q}' - \mathrm{C}\frac{\partial \mathrm{U}}{\partial x}\right) \qquad [10.42]$$

The vectors Y and Q" are introduced as:

$$\left.\begin{aligned} \mathrm{dY} &= \mathrm{K}^{-1}\mathrm{ds} \\ Q'' &= \mathrm{K}^{-1}\left(\mathrm{Q}' - \mathrm{C}\frac{\partial \mathrm{U}}{\partial x}\right) \end{aligned}\right\} \qquad [10.43]$$

Substituting definitions [10.43] into equation [10.42] leads to:

$$\frac{\partial \mathrm{Y}}{\partial t} + \Lambda\frac{\partial \mathrm{Y}}{\partial x} = \mathrm{Q}'' \qquad [10.44]$$

which is equivalent to:

$$\frac{\mathrm{d}Y_p}{\mathrm{d}t} = Q_p'' \qquad \text{for } \frac{\mathrm{d}x}{\mathrm{d}t} = \lambda^{(p)} \qquad [10.45]$$

The vector Y is the vector of sensitivity Riemann invariants. Note that Y can also be defined as:

$$\mathrm{Y} = \frac{\partial \mathrm{W}}{\partial \varphi} \qquad [10.46]$$

10.3.3. *The Riemann problem*

10.3.3.1. *Structure of the solution*

Consider the Riemann problem [10.21] defined for the hyperbolic part the governing equations. Recall that the solution of the Riemann problem is self-similar and that it verifies the following property (see Chapter 4):

$$\left(\mathrm{B}-\frac{x-x_0}{t}\mathrm{I}\right)\frac{\partial \mathrm{V}}{\partial x}=0 \qquad [10.47]$$

As shown in Chapter 4, equation [10.47] leads to Property (P4.3): the solution is made of m simple waves (rarefaction waves, shocks or contact discontinuities) separating regions of constant state. These waves originate from the location x_0 of the initial discontinuity.

The solution of the Riemann problem is determined uniquely from the left and right states provided that m independent relationships in s can be written across each wave. The next two sections focus on the derivation of such relationships for rarefaction waves and discontinuities.

10.3.3.2. *Rarefaction waves*

Assume that the pth wave is a rarefaction wave. Within this wave, $(x - x_0)/t$ is an eigenvalue for B, as indicated by equation [10.47]. Consequently, it is also an eigenvalue for A ($p = 1, \ldots, m$):

$$\lambda^{(p)}=\frac{x-x_0}{t} \qquad [10.48]$$

Differentiating equation [10.48] with respect to the parameter φ leads to:

$$\frac{\partial \lambda^{(p)}}{\partial \varphi}=0 \qquad [10.49]$$

Moreover, the Riemann invariants Y_q ($q \neq p$) provide $m - 1$ relationships:

$$Y_q=\frac{\partial W_q}{\partial \varphi}=\text{Const} \qquad \text{for}\ \frac{\mathrm{d}x}{\mathrm{d}t}\neq\lambda^{(p)}, q\neq p \qquad [10.50]$$

Consequently, m independent relationships are available across a rarefaction wave.

10.3.3.3. *Discontinuities*

If the *p*th wave is a shock or a contact discontinuity, the jump relationships [10.34] are applicable. However, both U and s being constant on each side of the wave in the solution of the Riemann problem, the space derivatives vanish in the expression of the source term R and the jump relationships are simplified into:

$$\left[\mathrm{s}^{(p,-)} - \mathrm{s}^{(p,+)}\right]\mathrm{c}_s = \mathrm{G}^{(p,-)} - \mathrm{G}^{(p,+)} - \left[\mathrm{U}^{(p,-)} - \mathrm{U}^{(p,+)}\right]\frac{\partial c_s}{\partial \varphi} \qquad [10.51]$$

where c_s is the speed of the discontinuity and superscripts $(p, -)$ and $(p, +)$ indicate respectively the values of the variables on the left- and right-hand side of the discontinuity. The expression for the derivative of c_s with respect to φ can be derived from the jump relationships for the variable U. Indeed, the Rankin-Hugoniot conditions yield:

$$c_s = \frac{F_q^{(p,-)} - F_q^{(p,+)}}{U_q^{(p,-)} - U_q^{(p,+)}} \qquad \forall q = 1, \ldots, m \qquad [10.52]$$

Consequently:

$$\frac{\partial c_s}{\partial \varphi} = \frac{G_q^{(p,-)} - G_q^{(p,+)}}{U_q^{(p,-)} - U_q^{(p,+)}} - \frac{\left[F_q^{(p,-)} - F_q^{(p,+)}\right]\left[s_q^{(p,-)} - s_q^{(p,+)}\right]}{\left[U_q^{(p,-)} - U_q^{(p,+)}\right]^2} \forall\, q = 1, \ldots, m \qquad [10.53]$$

Since $\partial c_s / \partial \varphi$ is entirely determined from the values of s and U on both sides of the discontinuity, m independent equations [10.51] can be written across a discontinuity.

10.3.4. *Application example: the one-dimensional shallow water sensitivity equations*

10.3.4.1. *Governing equations*

The purpose is to derive the analytical sensitivity solution for the dambreak problem presented in section 4.3.3. Recall that the dambreak problem is a Riemann problem under the assumption of zero bottom slope and frictionless motion.

If the channel is rectangular, the Saint Venant equations (see section 2.5) are equivalent to the one-dimensional version of the shallow water equations (see sections 5.4 and 7.4.2). U and F are defined as:

$$\mathrm{U} = \begin{bmatrix} h \\ q \end{bmatrix}, \mathrm{F} = \begin{bmatrix} q \\ M \end{bmatrix} = \begin{bmatrix} uh \\ q^2 / h + gh^2 / 2 \end{bmatrix} \quad [10.54]$$

where g is the gravitational acceleration, h is the water depth, M is the specific force, q is the unit discharge and u is the flow velocity.

The complete description of the solution of the dambreak problem is given in Chapter 4. Recall that the solution is made of an intermediate region of constant state separated from the let state by a rarefaction wave and from the right state by a shock. The Riemann invariant $W_2 = u + c$ is applicable across the rarefaction wave, while the jump relationships apply across the shock.

The Jacobian matrix A is recalled:

$$\mathrm{A} = \begin{bmatrix} 0 & 1 \\ c^2 - u^2 & 2u \end{bmatrix} \quad [10.55]$$

where $c = (gh)^{1/2}$ is the propagation speed of the waves in still water and $u = q/h$. The sensitivity vector s and the sensitivity flux G are defined as:

$$\mathrm{s} = \begin{bmatrix} \eta \\ \theta \end{bmatrix}, \qquad \mathrm{G} = \mathrm{As} = \begin{bmatrix} \theta \\ (c^2 - u^2)\eta + 2u\theta \end{bmatrix} \quad [10.56]$$

where η and θ are respectively the sensitivity of h and q to the parameter φ (that may be any parameter). The matrix B is given by:

$$\mathrm{B} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ c^2 - u^2 & 2u & 0 & 0 \\ 0 & 0 & 0 & 1 \\ (g - 2u^2 / h)\eta - 2u\theta / h & (\theta - u\eta) / h & c^2 - u^2 & 2u \end{bmatrix} \quad [10.57]$$

It is easy to check that B has the following double eigenvalues:

$$\left.\begin{aligned} \lambda^{(1)} &= \lambda^{(2)} = u - c \\ \lambda^{(3)} &= \lambda^{(4)} = u + c \end{aligned}\right\} \quad [10.58]$$

10.3.4.2. *Riemann problem definition*

The purpose is to solve the Riemann problem with left and right states in U:

$$\mathrm{U_L} = \begin{bmatrix} h_\mathrm{L} \\ 0 \end{bmatrix}, \qquad \mathrm{U_R} = \begin{bmatrix} h_\mathrm{R} \\ 0 \end{bmatrix} \tag{10.59}$$

with $h_\mathrm{L} > h_\mathrm{R}$.

The left and right states for the sensitivity depend on the parameter φ examined in the sensitivity analysis. In what follows, it is chosen to examine the sensitivity of the solution of the dambreak problem to the initial water level h_L on the left-hand side of the dam, while h_R is assumed fixed. Then $\varphi = h_\mathrm{L}$ and we have:

$$\mathrm{s_L} = \begin{bmatrix} \eta_\mathrm{L} \\ \theta_\mathrm{L} \end{bmatrix} = \begin{bmatrix} \partial h_\mathrm{L} / \partial h_\mathrm{L} \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \mathrm{s_R} = \begin{bmatrix} \eta_\mathrm{R} \\ \theta_\mathrm{R} \end{bmatrix} = \begin{bmatrix} \partial h_\mathrm{R} / \partial h_\mathrm{L} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{10.60}$$

Also note that if the sensitivity analysis focuses on the influence of initial or boundary conditions, the value of the parameter (the initial or boundary conditions) does not influence the expression of the flux F and source term S at times $t > 0$ within the domain. Therefore, $\partial \mathrm{F} / \partial \varphi = \partial \mathrm{S} / \partial \varphi = 0$ in the expression of the source term Q.

10.3.4.3. *Sensitivity solution*

In the rarefaction wave $\lambda^{(1)} = u - c$, equation [10.49] is applicable:

$$\upsilon - \chi = 0 \tag{10.61}$$

where υ and χ are respectively the sensitivity of u and c to the left state h_L. The speed c of the waves in still water is defined as $c = (gh)^{1/2}$.

Moreover, the Riemann invariant $W_2 = u + 2c$ may be used across the wave:

$$u + 2c = u_\mathrm{L} + 2c_\mathrm{L} \tag{10.62}$$

Differentiating equation [10.62] with respect to φ yields:

$$\upsilon + 2\chi = \upsilon_\mathrm{L} + 2\chi_\mathrm{L} \tag{10.63}$$

System [10.61–62] can be solved uniquely for υ and χ in the rarefaction wave:

$$\upsilon = \chi = \frac{\upsilon_{\mathrm{L}} + 2\chi_{\mathrm{L}}}{3} = \frac{2}{3}\chi_{\mathrm{L}} \text{ for } -c_L < \frac{x - x_0}{t} < u^* - c^* \qquad [10.64]$$

where the * superscript indicates the variables in the intermediate region of constant state. The sensitivities η and θ are derived from equation [10.64] by noting that $h = c^2/h$ and $q = hu$. Consequently:

$$\left.\begin{aligned} \eta &= \frac{2c}{g}\chi \\ \theta &= \eta u + h\upsilon \end{aligned}\right\} \qquad [10.65]$$

Applying the first equation [10.65] yields the expression for the left state c_{L} in equation [10.64]:

$$\chi_{\mathrm{L}} = \frac{g}{2c_{\mathrm{L}}}\eta_{\mathrm{L}} \qquad [10.66]$$

Moreover, the profile for c is given by equation [4.48], recalled here:

$$c(x,t) = \frac{1}{3}\left(2c_{\mathrm{L}} - \frac{x - x_0}{t}\right)$$

Substituting equations [10.64] and [4.48] into equation [10.65] leads to:

$$\eta(x,t) = \frac{2}{9c_{\mathrm{L}}}\left(2c_{\mathrm{L}} - \frac{x - x_0}{t}\right)\eta_{\mathrm{L}} \qquad \text{for } -c_L < \frac{x - x_0}{t} < u^* - c^* \qquad [10.67]$$

A similar reasoning yields the following expression for the sensitivity of the unit discharge:

$$\theta(x,t) = \frac{2\eta_{\mathrm{L}}}{9c_{\mathrm{L}}}\left(c_{\mathrm{L}} - \frac{x - x_0}{t}\right)\left(2c_{\mathrm{L}} + \frac{x - x_0}{t}\right) \text{ for } -c_L < \frac{x - x_0}{t} < u^* - c^* \qquad [10.68]$$

It is visible from equation [10.67] that the sensitivity of the water depth varies linearly with x in the rarefaction wave. In addition, using $(x - x_0)/t = -c_L$ in equation [10.67] yields a limit value $\eta = 2\eta_L/3$. Consequently, the sensitivity h is discontinuous at the left-hand boundary of the rarefaction wave. Equation [10.67] gives $\eta = 0$ for $(x - x_0)/t = 2\ c_L$ (Figure 10.4).

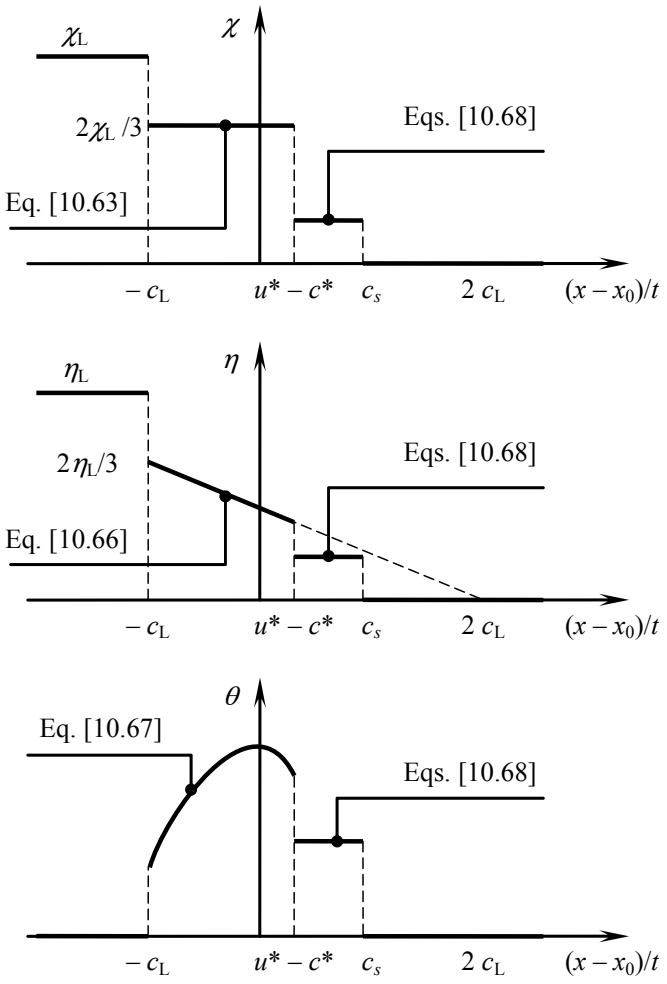

Figure 10.4. *Dambreak problem. Definition sketch for the sensitivity solution*

The sensitivities η^* and θ^* in the intermediate region of constant state are obtained by applying the jump relationships [10.51] and [10.53] and noting that $u_R = \eta_R = \theta_R = 0$:

$$\left.\begin{aligned} \eta^* \, c_s &= \theta^* - \eta^* \frac{\partial c_s}{\partial h_L} \\ \theta^* \, c_s &= (c^2 - u^2) * \eta^* + 2u * \theta^* - \theta^* \frac{\partial c_s}{\partial h_L} \end{aligned}\right\} \quad [10.69]$$

The shock speed c_s is known from the solution of the Riemann problem for the flow equations:

$$c_s = \frac{q^* - q_R}{h^* - h_R} = \frac{q^*}{h^* - h_R} \quad [10.70]$$

Differentiating with respect to $\varphi = h_L$ leads to:

$$\frac{\partial c_s}{\partial h_L} = \frac{\theta^*}{h^* - h_R} - \frac{q^* \eta^*}{(h^* - h_R)^2} \quad [10.71]$$

System [10.69–71] is nonlinear. It can be solved using iterative techniques such as Newton-Raphson's method. Note that in the general case, equations [10.69] and [10.67–68] do not yield a continuous sensitivity profile at the right-hand boundary of the rarefaction wave (Figure 10.4).

Figure 10.5 illustrates the solution obtained for the parameters in Table 10.1.

Symbol	Meaning	Value
g	Gravitational acceleration	9.81 m s^{-2}
h_L	Initial upstream water depth	10 m
h_R	Initial downstream water depth	1 m
η_L	Sensitivity to the initial water depth on the upstream side	1
η_R	Sensitivity to the initial water depth on the downstream side	0

Table 10.1. *Dambreak problem parameters*

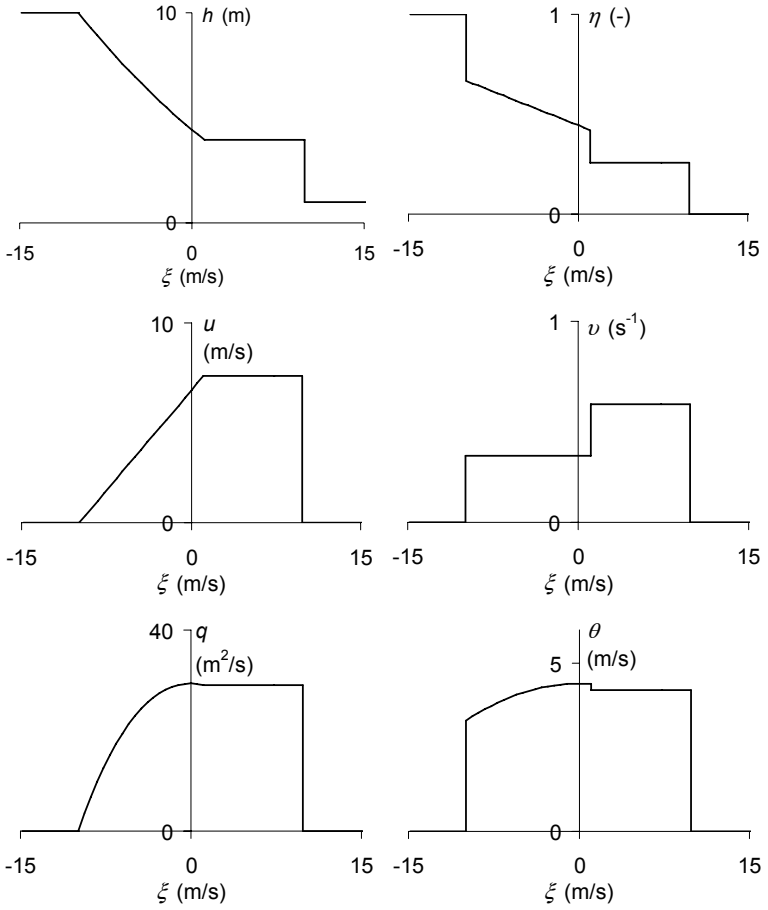

Figure 10.5. *Dambreak problem. Analytical solution for the parameter set in Table 10.1*

Figure 10.6 shows the empirical sensitivity profiles obtained from the numerical solution of the dambreak problem using a finite volume technique. The first-order Godunov scheme described in Chapter 7 is used with the HLL approximate Riemann solver described in Appendix C. The empirical sensitivity solution is computed by solving the shallow water equations twice. In the first simulation, the initial water depth on the left-hand side of the dam is set to $h_L + \varepsilon/2$. In the second simulation, it is set to $h_L - \varepsilon/2$. The sensitivities η, χ and θ are obtained by dividing the difference in h, c and q between the two simulations by ε.

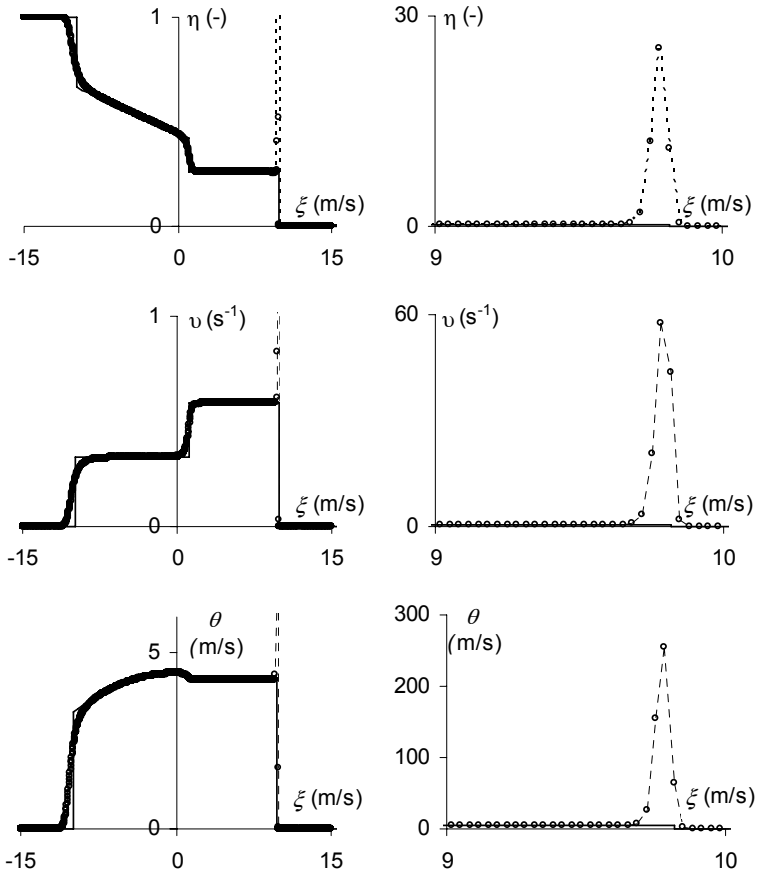

Figure 10.6. *Dambreak problem. Analytical solution (solid line) and empirical solution (dashed, dotted line) for the sensitivity*

The profiles are plotted as functions of the ratio $\xi = (x - x_0)/t$. The empirical sensitivity profiles clearly exhibit artificial peaks in the neighborhood of the shock. Rescaling the graph on the right-hand side of Figure 10.6 indicates that the amplitude of the artificial peak is up to 60 times that of the theoretical value of the sensitivity next to the shock. This example illustrates the need for numerical methods that do not exhibit such undesirable behaviors. Examples of such techniques are presented in section 10.5.

10.4. Adjoint sensitivity equations

10.4.1. *Introduction*

The forward sensitivity equations presented in the previous sections are most useful when the purpose of the sensitivity analysis is to study the influence of a single parameter on many model outputs (or variables). Examples of such situations are the sensitivity analysis of the dambreak problem presented in section 10.3.4. The influence of the upstream water level (a single simulation parameter) is studied for all the flow variables at all points and at all times.

In a number of inverse problems, however, the objective of the sensitivity analysis is to investigate the influence of numerous model parameters on a reduced set of flow variables. This is the case for instance when time-varying boundary conditions or spatially-varying initial conditions in a flow model are to be adjusted so as to reproduce flow measurements at a limited number of locations as accurately as possible. In this case, the number of points and time steps at which the initial and boundary conditions are to be adjusted may be much larger than the number of measurement points. The forward sensitivity approach is extremely time-consuming because it requires that one forward sensitivity calculation be carried out for each point (and each time) where the initial and/or boundary conditions are to be adjusted. In such situations, that are typical of inverse problems, the adjoint sensitivity analysis approach is more appropriate [CAC 03].

Adjoint sensitivity analysis is used in many fields of engineering such as model inversion (data assimilation [LED 86], model calibration, [PAN 89]), optimization problems, flow control and uncertainty analysis. Its earliest applications can be found in the field of meteorology and atmospheric sciences [HAL 82, HAL 83]. The reader interested in a formal, general definition of adjoint operators and an introduction to the underlying theory may refer to [CAC 03]. The theory of adjoint models can be found in [MAR 95]. The purpose of this section is to introduce the broad principles of adjoint sensitivity equations for one-dimensional hyperbolic conservation laws. The same derivation principle may be applied to systems of conservation laws. The reader interested in application examples of the adjoint sensitivity analysis technique to systems of conservation laws may refer to [SAN 00, SAN 99], which describe applications to free surface flow.

10.4.2. *Adjoint models for scalar laws*

10.4.2.1. *Derivation*

Consider a one-dimensional flow model obeying a scalar hyperbolic conservation law in the form [1.1], with a forward sensitivity equation in the

form [10.9]. For the sake of conciseness, the support function ε of the perturbation is considered to be uniformly zero and the solution is assumed to be continuous, therefore $R = 0$. It is also assumed that the wave speed λ is positive. The purpose is to optimize the value of the parameter φ so as to minimize a so-called objective function $J(\varphi)$ defined in general form as:

$$J(\varphi) = \int_0^T \int_0^L f(U, \varphi)\, \mathrm{d}x\, \mathrm{d}t \qquad [10.72]$$

where L and T are respectively the length of the domain and the time interval over which the objective function is defined. The parameter φ may be an initial or boundary condition, or a model parameter such as a friction coefficient, bottom slope (for an open channel model), sound speed or pipe diameter (for a water hammer model), etc. The function f depends on the nature of the optimization problem to be solved. Assume for instance that a measurement device provides an experimental value for U for a given time τ at a given abscissa X. No other measurement is available. If the purpose is to minimize the difference between the computed and measured value at $[X, \tau]$, the function f may be defined as a least square-based distance:

$$f(U, \varphi) = [U(X, \tau) - U_{\text{meas}}]^2 = \int_0^T \int_0^L [U(x, t) - U_{\text{meas}}]^2 \delta_{(X,\tau)} \mathrm{d}x\, \mathrm{d}t \qquad [10.73]$$

where $\delta_{(X, \tau)}$ is the Dirac function that takes effect at the abscissa X and time τ. The objective function J is zero (that is, minimum) when the distance between the simulated and measured variable U is zero.

Classically, gradient-based methods (sometimes called quasi-Newton methods) are used to find the minimum or zero of the objective function $J(\varphi)$. The gradient of J in the parameter space is given by:

$$\frac{\partial J}{\partial \varphi} = \int_0^T \int_0^L \frac{\partial f}{\partial \varphi} + \frac{\partial f}{\partial U}\frac{\partial U}{\partial \varphi}\, \mathrm{d}x\, \mathrm{d}t = \int_0^T \int_0^L \frac{\partial f}{\partial \varphi} + \frac{\partial f}{\partial U} s\, \mathrm{d}x\, \mathrm{d}t \qquad [10.74]$$

The expression of f being known, $\partial f / \partial \varphi$ and $\partial f / \partial U$ can be computed and the gradient of the objective function can be computed provided that the sensitivity s is known. However, as mentioned in the previous section, computing s for a large set of parameters φ is computationally expensive. The adjoint formulation is obtained

by modifying equation [10.74] as follows. The first equation [10.9] is rewritten as (note the simplification $\varepsilon = 0$, $R = 0$):

$$\frac{\partial s}{\partial t} + \frac{\partial G}{\partial x} - \frac{\partial S}{\partial U} s = 0 \qquad [10.75]$$

Equation [10.75] is multiplied by an arbitrary function $\mu(x, t)$ called the Lagrange multiplier. The resulting product, which is zero, is added to the integrand in equation [10.74], thus leading us to redefine the gradient of the objective function as:

$$\frac{\partial J}{\partial \varphi} = \int_0^T \int_0^L \left[\frac{\partial f}{\partial \varphi} + \frac{\partial f}{\partial U} s + \left(\frac{\partial \mathrm{s}}{\partial t} + \frac{\partial G}{\partial x} - \frac{\partial S}{\partial U} s \right) \mu \right] \mathrm{d}x \, \mathrm{d}t \qquad [10.76]$$

The adjoint equation is obtained by deriving a governing equation for the Lagrange multiplier μ. This is done via integration by parts:

$$\left.\begin{aligned} \int_0^T \int_0^L \frac{\partial s}{\partial t} \mu \, \mathrm{d}x \, \mathrm{d}t &= \int_0^L [s\mu]_0^T \, \mathrm{d}x - \int_0^T \int_0^L \frac{\partial \mu}{\partial t} s \, \mathrm{d}x \, \mathrm{d}t \\ \int_0^T \int_0^L \frac{\partial G}{\partial x} \mu \, \mathrm{d}x \, \mathrm{d}t &= \int_0^T [\mu G]_0^L \, \mathrm{d}t - \int_0^T \int_0^L \frac{\partial \mu}{\partial x} G \, \mathrm{d}x \, \mathrm{d}t \end{aligned}\right\} \qquad [10.77]$$

Substituting equations [10.77] into equation [10.76] and noting that $G = \lambda s$ leads to:

$$\begin{aligned} \frac{\partial J}{\partial \varphi} = &+ \int_0^L [\mu s]_0^T \, \mathrm{d}x + \int_0^T [\mu G]_0^L \, \mathrm{d}t + \int_0^T \int_0^L \frac{\partial f}{\partial \varphi} \mathrm{d}x \, \mathrm{d}t \\ &- \int_0^T \int_0^L \left(\frac{\partial \mu}{\partial t} + \lambda \frac{\partial \mu}{\partial x} + \frac{\partial S}{\partial U} \mu - \frac{\partial f}{\partial U} \right) s \, \mathrm{d}x \, \mathrm{d}t \end{aligned} \qquad [10.78]$$

Assume that μ verifies the following equation:

$$\frac{\partial \mu}{\partial t} + \lambda \frac{\partial \mu}{\partial x} + \frac{\partial S}{\partial U} \mu - \frac{\partial f}{\partial U} = 0 \qquad [10.79]$$

Equation [10.79] is similar to equation [10.75], with the difference that (i) an additional term $\partial f / \partial U$ is introduced and (ii) the sign of the source term $\partial S / \partial U$ is

changed. This has consequences on the stability of μ. The solution s of equation [10.75] is stable when computed for increasing times. Changing the sign of the term $\partial S/\partial U$ in equation [10.79] may result in instability if μ is also computed for increasing times. The initial sign for the source term can be recovered by introducing the reverse time and space coordinates $t' = T - t$ and $x' = L - x$. Equation [10.79] becomes:

$$\frac{\partial \mu}{\partial t'} + \lambda \frac{\partial \mu}{\partial x'} = \frac{\partial S}{\partial U}\mu + \frac{\partial f}{\partial U} \qquad [10.80]$$

This is the final form of the adjoint sensitivity equation. The solution μ is stable if computed in the direction of positive t', that is, for negative t. Assuming that λ is positive, a boundary condition is needed at $x' = 0$ (that is, at $x = L$). The initial condition is needed for $t' = 0$ (which corresponds to $t = T$). The simplest possible conditions are:

$$\left.\begin{aligned} \mu(x,T) &= 0 \qquad \forall x \in [0,L] \\ \mu(L,t) &= 0 \qquad \forall t \in [0,T] \end{aligned}\right\} \qquad [10.81]$$

Assuming that the adjoint equation [10.80] with initial and boundary conditions [10.81] is satisfied, substituting equations [10.79] and [10.81] into equation [10.78] leads to the following expression for the gradient of the objective function:

$$\begin{aligned} \frac{\partial J}{\partial \varphi} &= -\int_0^L (\mu s)(x,0)\,\mathrm{d}x - \int_0^T (\mu G)(0,t)\,\mathrm{d}t + \int_0^T \int_0^L \frac{\partial f}{\partial \varphi}\,\mathrm{d}x\,\mathrm{d}t \\ &= -\int_0^L (s\mu)(x,0)\,\mathrm{d}x - \int_0^T (\lambda s\mu)(0,t)\,\mathrm{d}t + \int_0^T \int_0^L \frac{\partial f}{\partial \varphi}\,\mathrm{d}x\,\mathrm{d}t \end{aligned} \qquad [10.82]$$

10.4.2.2. *Physical interpretation – algorithmic aspects*

The adjoint equation [10.80] may be interpreted as follows: the origin of a perturbation in the variable U at a given location (x, t) in the solution domain is to be sought at earlier times, at the points the perturbation is likely to come from. Solving equation [10.80] is equivalent to traveling backward along the characteristic lines in the (x, t) plane (Figure 10.7). The smaller the value of μ at $t = 0$ and/or $x = 0$, the smaller the value of the integrals in equation [10.82], thus the smaller the magnitude of $\partial J/\partial \varphi$. The Lagrange multiplier may be seen as an indicator of the influence of the flow solution at a given time and abscissa on the final value of the objective function.

From an algorithmic point of view, the adjoint formalism associated with a quasi-Newton procedure implies the following steps:

(1) Forward step: solve the flow and forward sensitivity equation in the direction of positive time over the interval [0, T] for a given value of the parameter φ. This provides the value of U and s. The objective function J is computed from equation [10.72]. In the general case, J is not minimum for the selected value of φ.

(2) Backward step: solve the adjoint sensitivity equation [10.80] with initial and boundary conditions [10.81] in the direction of negative times. This yields the Lagrange multiplier μ at all points (x, t) of the solution domain [0, L]×[0, T].

(3) Compute the gradient $\partial J / \partial \varphi$ using equation [10.82]. Update the parameter φ using a classical Newton procedure:

$$\varphi \mapsto \varphi - \frac{J(\varphi)}{\partial J / \partial \varphi} \qquad [10.83]$$

Steps (1) – (3) are repeated sequentially.

In practical computer implementations, the sequence (1) – (2) involves that the results of the forward flow and sensitivity calculation being stored and available for the backward solution of the adjoint problem. In contrast with the classical forward computation procedure, the previously computed time levels cannot be erased from the memory of the computer because the flow variables must be available over the entire time interval [0, T]. This may imply considerable memory and storage requirements.

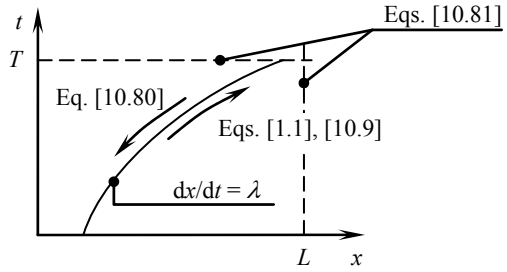

Figure 10.7. *Forward and adjoint sensitivity equations. Definition sketch in the (x, t) plane*

10.4.2.3. *Extension to hyperbolic systems*

The adjoint sensitivity system is derived as follows. Each component of the vector sensitivity equation is multiplied by a Lagrange multiplier μ_p:

$$\left(\frac{\partial s_p}{\partial t}+\frac{\partial G_p}{\partial x}-Q_p\right)\mu_p=0, \qquad p=1,\ldots,m \qquad [10.84]$$

where subscript p denotes the component of the vector equation. Adding this system to the objective function as in section 10.4.2.1 leads to:

$$\frac{\partial \mathrm{s}_\Delta}{\partial t}\mathrm{M}+\frac{\partial \mathrm{G}_\Delta}{\partial x}\mathrm{M}-\mathrm{Q}_\Delta\mathrm{M}-\frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M}=0 \qquad [10.85]$$

where M is the vector of Lagrange multipliers and s_Δ, G_Δ and Q_Δ are diagonal matrices constructed from the components of the vectors s, G and Q:

$$\mathrm{s}_\Delta=\begin{bmatrix}\ddots & & 0\\ & s_p & \\ 0 & & \ddots\end{bmatrix},\quad \mathrm{G}_\Delta=\begin{bmatrix}\ddots & & 0\\ & G_p & \\ 0 & & \ddots\end{bmatrix},\quad \mathrm{Q}_\Delta=\begin{bmatrix}\ddots & & 0\\ & Q_p & \\ 0 & & \ddots\end{bmatrix} \qquad [10.86]$$

As in section 10.4.2.1, the differential operators are swapped via integration by parts, leading to the following equation:

$$\mathrm{s}_\Delta\frac{\partial \mathrm{M}}{\partial t'}+\mathrm{G}_\Delta\frac{\partial \mathrm{M}}{\partial x'}=\mathrm{Q}_\Delta\mathrm{M}+\frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M} \qquad [10.87]$$

Multiplying equation [10.87] by the inverse of s_Δ leads to the adjoint system:

$$\frac{\partial \mathrm{M}}{\partial t'}+\mathrm{s}_\Delta^{-1}\mathrm{G}_\Delta\frac{\partial \mathrm{M}}{\partial x'}=\mathrm{s}_\Delta^{-1}\mathrm{Q}_\Delta\mathrm{M}+\mathrm{s}_\Delta^{-1}\frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M} \qquad [10.88]$$

Riemann invariants can be derived for the Lagrange multipliers. Left-multiplying equation [10.88] by K^{-1} leads to:

$$\frac{\partial \psi}{\partial t'}+\Lambda\frac{\partial \psi}{\partial x'}=\mathrm{K}_\Delta^{-1}\left(\mathrm{s}_\Delta^{-1}\mathrm{Q}_\Delta\mathrm{M}+\mathrm{s}_\Delta^{-1}\frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M}\right) \qquad [10.89]$$

where K_Δ is the matrix of eigenvectors of $\mathrm{s}_\Delta^{-1}\mathrm{G}_\Delta$ and ψ is the vector of adjoint Riemann invariants:

$$\mathrm{d}\psi=\mathrm{K}_\Delta^{-1}\,\mathrm{dM} \qquad [10.90]$$

A more convenient way of deriving the characteristic form of the adjoint equation consists of starting from the characteristic form [10.44] of the sensitivity equation:

$$\frac{\partial \mathrm{Y}_\Delta}{\partial t}\mathrm{M} + \Lambda \frac{\partial \mathrm{Y}_\Delta}{\partial x}\mathrm{M} = \mathrm{Q}''_\Delta \mathrm{M} + \frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M} \qquad [10.91]$$

Applying integration by parts yields the adjoint equation:

$$\mathrm{Y}_\Delta \frac{\partial \mathrm{M}}{\partial t'} + \Lambda\, \mathrm{Y}_\Delta \frac{\partial \mathrm{M}}{\partial x'} = \mathrm{Q}^{(3)} + \frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M} \qquad [10.92]$$

where $\mathrm{Q}^{(3)} = \mathrm{Q}''_\Delta \mathrm{M}$. Multiplying by the inverse of Y_Δ and noting that $\mathrm{Y}_\Delta^{-1}\, \Lambda\, \mathrm{Y}_\Delta = \Lambda$ leads to:

$$\frac{\partial \mathrm{M}}{\partial t'} + \Lambda \frac{\partial \mathrm{M}}{\partial x'} = \mathrm{Y}_\Delta^{-1}\left(\mathrm{Q}^{(3)} + \frac{\partial \mathrm{f}}{\partial \mathrm{U}}\mathrm{M} \right) \qquad [10.93]$$

The vector equation [10.93] forms a system of *m* characteristic equations. The Lagrange multipliers μ_p ($p = 1, \ldots, m$) are the adjoint Riemann invariants.

10.5. Finite volume solution of the forward sensitivity equations

10.5.1. *Introduction*

As shown in section 10.3.4, the empirical solution of sensitivity equations yields numerical artifacts such as abnormally large (if not locally infinite) values of the computed sensitivity. Other artifacts have been observed in two-dimensional free surface flow simulations, such as artificial sensitivity swirls in regions where they should not be present [GUI 09c]. Such artifacts can be eliminated to a large extent if the sensitivity equations are solved directly.

Most methods for direct sensitivity calculation presented in the literature deal with continuous solutions (see e.g. [GUN 99, LU 07]). The purpose of this section is to provide the broad lines for a finite volume-based solution technique of sensitivity equations with discontinuous flow solutions. The principle of the method is presented in [GUI 07] for scalar laws, with an application to the kinematic wave model seen in Chapter 1.

The technique is extended to the shallow water equations in [DEL 08, GUI 09c]. A more accurate version of the Riemann solver with an extension to 3×3 systems including a passive scalar transport equation is given in [GUI 09a, GUI 09b].

Practical implementation aspects, including boundary conditions, can be found in [GUI 09b].

10.5.2. *Discretization*

The purpose is to solve the $2m \times 2m$ hyperbolic system [10.35] formed by the governing equations for the flow variable U and the sensitivity s. For the sake of clarity, only the case $m = 2$ is considered and the source terms S and Q are assumed to be zero. Consequently, the vector source term T as defined in equation [10.36] only incorporates the sensitivity Dirac source term at discontinuities. A finite volume discretization is proposed in [DEL 08, GUI 09a, GUI 09b, GUI 09c] (Figure 10.8):

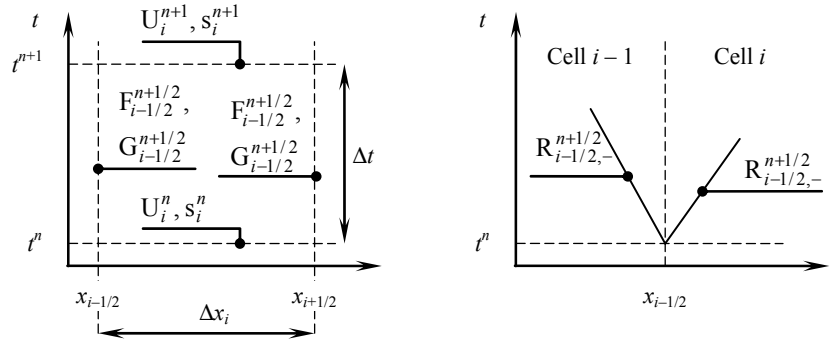

Figure 10.8. *Direct solution of the sensitivity equations. Definition sketch for the finite volume solution technique. Left: principle of the finite volume discretization. Right: splitting the sensitivity source term into two parts at each interface*

$$\left.\begin{aligned} U_i^{n+1} &= U_i^n + \frac{\Delta t}{\Delta x_i}(F_{i-1/2}^{n+1/2} - F_{i+1/2}^{n+1/2}) \\ s_i^{n+1} &= s_i^n + \frac{\Delta t}{\Delta x_i}(G_{i-1/2}^{n+1/2} - G_{i+1/2}^{n+1/2} + R_{i-1/2,+}^{n+1/2} + R_{i+1/2,-}^{n+1/2}) \end{aligned}\right\} \qquad [10.94]$$

where subscripts i, $i - 1/2$ and $i + 1/2$ indicate respectively the average value in the cell i , the value at the interfaces $i - 1/2$ and $i + 1/2$, and superscripts n and $n + 1/2$ denote respectively the value at the time level n and the average value between the time levels n and $n + 1$. Subscript $(i - 1/2, +)$ denotes the contribution of the source term R arising from interface $i - 1/2$ to the cell located in the direction of positive x (that is, cell i). Conversely, subscript $(i + 1/2, -)$ denotes the contribution of the source term arising from interface $i + 1/2$ to the cell located on the left-hand side (that is, cell i).

F, G and R are estimated from the solution of Riemann problems at the interfaces between the computational cells. The contributions $R_{i-1/2,-}^{n+1/2}$ and $R_{i-1/2,+}^{n+1/2}$ shown in Figure 10.8 are computed from the solution of the Riemann problem. $R_{i-1/2,-}^{n+1/2}$ arises from the waves with negative propagation speeds, while $R_{i-1/2,+}^{n+1/2}$ is associated with waves that have a positive propagation speeds. The proposed approach being explicit, the estimates of F, G and R in equations [10.94] are based on the values of U, s, F and G at the known time level n.

10.5.3. *A modified HLL Riemann solver for sensitivity solutions*

10.5.3.1. *Principle of the solver*

The fluxes $F_{i-1/2}^{n+1/2}$ and $G_{i-1/2}^{n+1/2}$ at the interface $i-1/2$ are computed by solving a Riemann problem with left and right states V_L and V_R. If the first-order Godunov scheme is used, V_L and V_R are respectively equal to the average values in the cells $i-1$ and i. If higher-order schemes are used, V_L and V_R are inferred from the reconstructed profiles in the cells $i-1$ and i. The states V_L and V_R are assumed known hereafter.

The Riemann solver proposed in [GUI 09a, GUI 09b] is an extension of the approximate HLL Riemann solver described in Appendix C (see section C.1). Recall that the HLL Riemann solver uses the assumption of an intermediate region of constant state (U*, s*) separated from the left and right states of the Riemann problem by two discontinuities. The jump relationships hold across these discontinuities:

$$\left.\begin{aligned} F_L - F^* &= (U_L - U^*)\,\lambda^{(1)} \\ F^* - F_R &= (U^* - U_R)\,\lambda^{(2)} \\ G_L - G^* &= (s_L - s^*)\,\lambda^{(1)} + (U_L - U^*)\frac{\partial \lambda^{(1)}}{\partial \varphi} \\ G^* - G_R &= (s^* - s_R)\,\lambda^{(2)} + (U^* - U_R)\frac{\partial \lambda^{(2)}}{\partial \varphi} \end{aligned}\right\} \qquad [10.95]$$

where $\lambda^{(1)}$ and $\lambda^{(2)}$ are the speeds of the left- and right-hand discontinuities. These speeds are assumed known *a priori* from the left and right states. Various estimates for them are provided in Appendix C. Note that the jump relationships for the sensitivity in [10.95] are obtained as particular cases of the more general jump relationships [10.34] because the x-derivatives of the HLL-solution are zero.

10.5.3.2. *Flux formulae*

System [10.94] can be solved uniquely for U*, s*, F* and G*:

$$\left.\begin{aligned}
U^* &= \frac{-\lambda^{(1)}U_L + \lambda^{(2)}U_R}{\lambda^{(2)} - \lambda^{(1)}} + \frac{F_L - F_R}{\lambda^{(2)} - \lambda^{(1)}} \\
F^* &= \frac{\lambda^{(2)}F_L - \lambda^{(1)}F_R}{\lambda^{(2)} - \lambda^{(1)}} - \frac{\lambda^{(1)}\lambda^{(2)}}{\lambda^{(2)} - \lambda^{(1)}}(U_L - U_R) \\
s^* &= \frac{-\lambda^{(1)}s_L + \lambda^{(2)}s_R}{\lambda^{(2)} - \lambda^{(1)}} + \frac{G_L - G_R}{\lambda^{(2)} - \lambda^{(1)}} \\
&\quad + \frac{1}{\lambda^{(2)} - \lambda^{(1)}}\frac{\partial\lambda^{(2)}}{\partial\varphi}(U^* - U_R) + \frac{1}{\lambda^{(2)} - \lambda^{(1)}}\frac{\partial\lambda^{(1)}}{\partial\varphi}(U_L - U^*) \\
G^* &= \frac{\lambda^{(2)}G_L - \lambda^{(1)}G_R}{\lambda^{(2)} - \lambda^{(1)}} - \frac{\lambda^{(1)}\lambda^{(2)}}{\lambda^{(2)} - \lambda^{(1)}}(s_L - s_R) \\
&\quad + \frac{\lambda^{(1)}}{\lambda^{(2)} - \lambda^{(1)}}\frac{\partial\lambda^{(2)}}{\partial\varphi}(U^* - U_R) + \frac{\lambda^{(2)}}{\lambda^{(2)} - \lambda^{(1)}}\frac{\partial\lambda^{(1)}}{\partial\varphi}(U_L - U^*)
\end{aligned}\right\} \quad [10.96]$$

The second equation [10.96] provides the expression for the flux F* in the intermediate region of constant state. The flux at the interface $i - 1/2$ is equal to F_L if $\lambda^{(1)} > 0$, to F* if $\lambda^{(1)} \leq 0 \leq \lambda^{(2)}$, and to F_R if $\lambda^{(2)} < 0$. These three formulae can be gathered into a single expression as:

$$F_{i-1/2}^{n+1/2} = \frac{\lambda^+ F_L - \lambda^- F_R}{\lambda^+ - \lambda^-} - \frac{\lambda^-\lambda^+}{\lambda^+ - \lambda^-}(U_L - U_R) \quad [10.97]$$

where λ^- and λ^+ are bounded expressions for $\lambda^{(1)}$ and $\lambda^{(2)}$:

$$\left.\begin{aligned}
\lambda^- &= \min(\lambda^{(1)}, 0) \\
\lambda^- &= \max(\lambda^{(2)}, 0)
\end{aligned}\right\} \quad [10.98]$$

A similar expression can be proposed for $G_{i-1/2}^{n+1/2}$:

$$\begin{aligned}
G^* &= \frac{\lambda^+ G_L - \lambda^- G_R}{\lambda^+ - \lambda^-} - \frac{\lambda^-\lambda^+}{\lambda^+ - \lambda^-}(s_L - s_R) \\
&\quad + \frac{\lambda^-}{\lambda^+ - \lambda^-}\frac{\partial\lambda^+}{\partial\varphi}(U^* - U_R) + \frac{\lambda^+}{\lambda^+ - \lambda^-}\frac{\partial\lambda^-}{\partial\varphi}(U_L - U^*)
\end{aligned} \quad [10.99]$$

In contrast with equation [10.97], equation [10.99] requires that the intermediate state U* in the intermediate region of constant state be computed. This is done using the first equation [10.96]. Note that in this equation, $\lambda^{(1)}$ and $\lambda^{(2)}$ must not be replaced with λ^- and λ^+, the role of which is only to provide a unified formula to handle the subcritical/supercritical transition at the interface.

A pending question is the expression of the derivatives $\partial\lambda^{\pm}/\partial\varphi$ in equation [10.99]. As proposed in [GUI 09a, GUI 09b], these derivatives are computed by noting that λ^- and λ^+ are known functions of the left and right states U_L and U_R:

$$\frac{\partial\lambda^{\pm}}{\partial\varphi}=\frac{\partial\lambda^{\pm}}{\partial U_L}\frac{\partial U_L}{\partial\varphi}+\frac{\partial\lambda^{\pm}}{\partial U_R}\frac{\partial U_R}{\partial\varphi}=\frac{\partial\lambda^{\pm}}{\partial U_L}s_L+\frac{\partial\lambda^{\pm}}{\partial U_R}s_R \qquad [10.100]$$

The derivatives $\partial\lambda^{\pm}/\partial U_L$ and $\partial\lambda^{\pm}/\partial U_R$ are row vectors. Their product with the column vectors s_L and s_R gives a scalar quantity.

10.5.3.3. *Dirac source term*

The discretization of the Dirac source term R is examined. The source term $R_{i-1/2,-}^{n+1/2}$ is given by:

$$R_{i-1/2,-}^{n+1/2}=\begin{cases}\beta_1\dfrac{\partial\lambda^{(1)}}{\partial\varphi}(s_L-s^*)+\beta_2\dfrac{\partial\lambda^{(2)}}{\partial\varphi}(s^*-s_R) & \text{if } \lambda^{(2)}<0\\ \beta_1\dfrac{\partial\lambda^{(1)}}{\partial\varphi}(s_L-s^*) & \text{if } \lambda^{(1)}<0<\lambda^{(2)}\\ 0 & \text{if } \lambda^{(1)}>0\end{cases} \qquad [10.101]$$

where β_1 and β_2 are indicators, $\beta_p=1$ if the wave p is a shock or contact discontinuity, $\beta_p=0$ otherwise. Conversely, the source term $R_{i-1/2,+}^{n+1/2}$ is given by:

$$R_{i-1/2,+}^{n+1/2}=\begin{cases}0 & \text{if } \lambda^{(2)}<0\\ \beta_2\dfrac{\partial\lambda^{(2)}}{\partial\varphi}(s^*-s_R) & \text{if } \lambda^{(1)}<0<\lambda^{(2)}\\ \beta_1\dfrac{\partial\lambda^{(1)}}{\partial\varphi}(s_L-s^*)+\beta_2\dfrac{\partial\lambda^{(2)}}{\partial\varphi}(s^*-s_R) & \text{if } \lambda^{(1)}>0\end{cases} \qquad [10.102]$$

The following criterion is used for shock detection [GUI 09a, GUI 09b]:

$$\left.\begin{aligned} \beta_1 = 1 \quad \text{if} \begin{cases} \lambda^{(1)}(\mathrm{U_L}) > \lambda^{(1)}(\mathrm{U^*}) \\ \lambda^{(2)}(\mathrm{U_L}) > \lambda^{(2)}(\mathrm{U^*}) \end{cases} \\ \beta_2 = 1 \quad \text{if} \begin{cases} \lambda^{(1)}(\mathrm{U^*}) > \lambda^{(1)}(\mathrm{U_R}) \\ \lambda^{(2)}(\mathrm{U^*}) > \lambda^{(2)}(\mathrm{U_R}) \end{cases} \end{aligned}\right\} \qquad [10.103]$$

10.5.4. *Application example: the one-dimensional shallow water equations*

The sensitivity Riemann solver is applied to the dambreak problem presented in section 10.3.4, with the parameters given in Table 10.1. More details can be found on the analytical solution of this problem and extensions to constant bottom slopes in [GUI 09a-c].

The numerical solution is computed over a domain discretized into 1,000 cells of width 1 m. The computational time step is set to the maximum permissible value given by the stability constraint $(u + c)\,\Delta t_{\max} = \Delta x$. Figure 10.9 shows the analytical and numerical solution for the sensitivity variables η, χ, υ and θ. In contrast with the empirical solution shown in Figure 10.6, there is no artificial peak in the solution computed by the sensitivity solver.

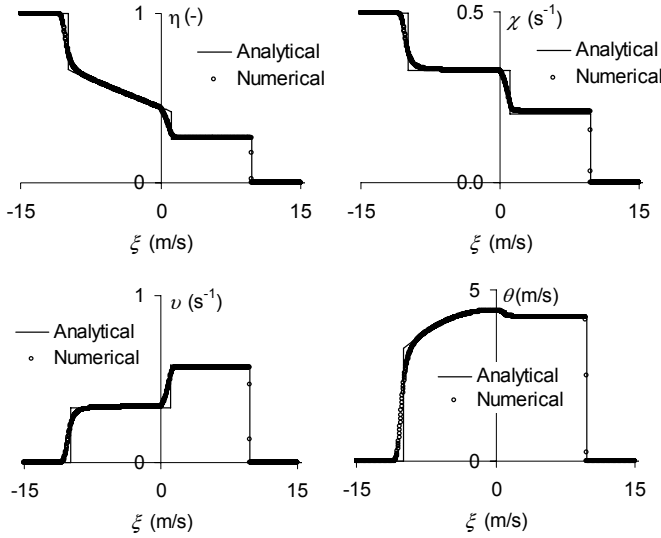

Figure 10.9. *Dambreak problem. Analytical solution and numerical solution obtained using the modified HLL solver*

10.6. Summary

Sensitivity equations for hyperbolic conservation laws or hyperbolic systems are obtained by differentiating the flow governing equations with respect to the parameter of interest. This parameter may be an initial condition, a boundary condition, or a parameter in the flux and/or in the source term. The sensitivity equations can be formulated in forward form (see sections 10.2 and 10.3) and in adjoint form (see section 10.4).

The wave speed of the sensitivity system are identical to the wave speeds of the flow system (sections 10.2 and 10.3). Consequently, the system formed by the flow equations and their sensitivity equations is not strictly hyperbolic but linearly degenerate because all the eigenvalues in the system are double eigenvalues. In the adjoint formulation, invariants can be defined for the Lagrange multipliers. The wave propagation speeds of these adjoint Riemann invariants are identical to those of the flow system. The adjoint invariants are calculated by following the characteristics in the backward time direction.

Discontinuous flow solutions generate Dirac sensitivity source terms that take effect at the flow discontinuities (sections 10.2.3 and 10.3.3). The jump relationships for the sensitivity are given by equation [10.19]. In the solution of the Riemann problem (sections 10.2.4 and 10.3.3), the sensitivity is discontinuous at the edges of rarefaction waves. In the solution of the Riemann problem for scalar conservation laws, rarefaction waves are zero sensitivity regions. The analytical sensitivity solution of the dambreak problem for the Saint Venant equations is derived in section 10.3.4.

Numerical methods are available for the discretization of the forward sensitivity equations in the presence of discontinuous solutions. A modified HLL Riemann solver is presented in section 10.5, with an application to the dambreak problem derived in section 10.3.4.