

AN ALTERNATIVE PROCEDURE FOR SIMULATING A CLASS OF HYPERBOLIC SYSTEMS

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Abstract. This work presents an alternative numerical procedure for simulating nonlinear hyperbolic systems, using Glimm's method for advancing in time. The standard procedure to implement this methodology suffers from the disadvantage of requiring a complete solution of the associated Riemann problem – a task, in general, not easily reached. The alternative procedure introduced in this article consists in approximating the solution of the associated Riemann problem by piecewise constant functions always satisfying the jump condition – thus circumventing the difficulty of solving the Riemann problem and giving rise to an approximation easier to implement with lower computational cost. In order to illustrate the good performance of the alternative methodology proposed, the transport of a pollutant in an environment representing an atmosphere is simulated. Comparison with the standard procedure, employing the complete solution of the associated Riemann problem for implementing Glimm's scheme, has shown good agreement.

Keywords. Glimm's scheme, Riemann solver, shock waves, pollutant transport.

1. Introduction

Most transport phenomena description involve parabolic or elliptic partial differential equations which always admit regular solutions whose simulation may employ well known numerical tools like finite elements, finite differences or finite volumes. Hyperbolic systems, on the other hand, allow very realistic descriptions, since the propagation of any quantity – or information – in real natural phenomena is characterized by a finite speed. Glimm's scheme – a reliable method for simulating hyperbolic systems whose accuracy is mathematically ensured (Glimm, 1965; Chorin, 1976) is based on a theory presenting a solid thermodynamic basis (Smoller, 1983). Two important features of this numerical scheme, actually the scheme that better preserves the shock identity among the numerical procedures adequate to cope with discontinuous problems, deserve a special remark. First, if the width of the steps tends to zero, the approximation obtained by Glimm's method tends to the exact solution of the problem – considering its weak formulation. Another characteristic of this scheme is that it does not dissipate shocks, preserving their magnitude (no diffusion being observed) and position. Nevertheless, the standard procedure for its implementation – when simulating problems with any initial data and/or boundary condition – suffers from the disadvantage of requiring previous knowledge of the complete solution of the Riemann problem associated with the hyperbolic system, since Glimm's method approximates hyperbolic nonlinear problems by appropriately gathering the solution of a certain number of associated Riemann problems. The determination of the complete solution of the associated Riemann problem, besides its inherent difficulty, renders the computational implementation more expensive.

This article is focused on the proposition of a Riemann solver allowing to build a simple and efficient procedure for simulating hyperbolic systems circumventing the requirement of a complete solution for the associated Riemann problem. This solution is approximated by piecewise constant functions satisfying the jump conditions, but not necessarily the entropy condition. The above-mentioned procedure, associated with Glimm's scheme, provides a convenient way for simulating hyperbolic systems. Simulations of the transport of a pollutant in the atmosphere exemplify the methodology.

The simplified mathematical modeling for the transport of a pollutant in the air employed in this work combines the mass and linear momentum balances for the air-pollutant mixture – the classical equations of gas dynamics – with the pollutant mass balance, giving rise to a nonlinear system of hyperbolic partial differential equations presenting discontinuities – which will be shock waves in case they satisfy the entropy condition – in addition to classical solutions. Besides, this genuinely nonlinear hyperbolic resulting problem presents a very interesting feature – a contact shock characterized by presenting the same speed of the second eigenvalue. Along this shock there is a jump in the

pollutant concentration but, on the other hand, the mass density and the velocity remain constant, i.e. they do not jump (Martins-Costa and Saldanha da Gama, 2003).

2. Mechanical model

The transport of a pollutant in the air is described by considering a simplified model based on the mass and linear momentum conservation for the air-pollutant mixture and the mass balance for the pollutant along with some hypotheses. First the mass transfer is supposed to be caused by an advection process of the pollutant – from now on denoted as A constituent – in the air, which is assumed as an ideal gas (all viscosity effects being neglected). Diffusion will be neglected, when compared to advection. Also, supposing the presence of a sufficiently small quantity of the constituent A in the air – at any time instant, along with mass densities with the same order of magnitude for both air and the A constituent, the mass and linear momentum balance equations for the mixture can be approximated by mass and linear momentum balances for the air. Additional simplifying assumptions are absence of chemical reactions which could alter the quantity of the constituent A and the pressure acting on the air being p considered as a function of the air mass density ρ only, its derivative satisfying $\hat{p}'(\rho) > 0$. Finally, a plane horizontal flow is considered so that the air velocity field \mathbf{v} may be reduced to a single component on the flow direction $\mathbf{v} = v\mathbf{i}$ and gravitational effects may be omitted. Considering all the above stated hypotheses, the transport of a pollutant in the air is mathematically described by the following nonlinear homogeneous hyperbolic system

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) &= 0 \\ \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho v^2 + p) &= 0 \\ \frac{\partial}{\partial t}(\rho \omega_A) + \frac{\partial}{\partial x}(\rho \omega_A v) &= 0 \end{aligned} \quad (1)$$

in which ω_A represents the pollutant concentration in the mixture, expressed by the ratio between the pollutant mass density and the mixture (or air) mass density. Defining the following dimensionless quantities

$$\eta = \frac{x}{L} \quad \tau = \frac{t\tilde{v}}{L} \quad \tilde{\rho} = \frac{\rho}{\tilde{\rho}} \quad \tilde{v} = \frac{v}{\tilde{v}} \quad \tilde{p} = \frac{p}{\tilde{\rho}\tilde{v}^2} \quad (2)$$

in which L is a reference length, \tilde{v} a reference velocity and $\tilde{\rho}$ a reference mass density. Now, the following redefinition of variables is considered: $F \equiv \tilde{\rho}$, $G \equiv \tilde{\rho}\tilde{v}$, $H \equiv \tilde{\rho}\omega_A$. So problem (1), which is subjected to a given data at $t = t_n$ ($F = \hat{F}_n(x)$, $G = \hat{G}_n(x)$ and $H = \hat{H}_n(x)$ at $t = t_n$) is rewritten as

$$\begin{aligned} \frac{\partial F}{\partial \tau} + \frac{\partial G}{\partial \eta} &= 0 \\ \frac{\partial G}{\partial \tau} + \frac{\partial}{\partial \eta} \left(\frac{G^2}{F} + \tilde{p}(F) \right) &= 0 \\ \frac{\partial H}{\partial \tau} + \frac{\partial}{\partial \eta} \left(\frac{GH}{F} \right) &= 0 \end{aligned} \quad (3)$$

3. Numerical approximation

Considering the Riemann problem associated with the hyperbolic system (3), its generalized solution is reached by connecting the left (L) and right (R) states by means of two intermediate constant states (*1 and *2) as follows: $(F_L, G_L, H_L) \rightarrow (F_{*1}, G_{*1}, H_{*1}) \rightarrow (F_{*2}, G_{*2}, H_{*2}) \rightarrow (F_R, G_R, H_R)$. The connection between the states $L \rightarrow *1$, $*1 \rightarrow *2$ and $*2 \rightarrow R$ may be performed either by rarefactions or shocks. A particular type of link is verified in the Riemann problem associated to (1) – the connection between intermediate states *1 and *2 is always a contact shock, where there is no jump for both variables F and G – in such a way that $F_{*1} = F_{*2}$ and $G_{*1} = G_{*2}$. The jump is verified solely for H , with a propagation speed G/F . A contact shock may be viewed as the limiting case of a rarefaction in which the rarefaction fan is reduced to a single line; namely a discontinuity with associated eigenvalue corresponding exactly to the shock speed (Martins-Costa and Saldanha da Gama, 2003).

System (3) is approximated by employing Glimm's scheme, described in details in Martins-Costa and Saldanha da Gama (2003), to advance from time τ_n to time τ_{n+1} . Glimm's method for building a solution for an initial value

problem consists in appropriately gathering the solution of a certain previously chosen number of Riemann problems to successively march from time $\tau = \tau_n$ to time $\tau_{n+1} = \tau_n + \Delta\tau$. The arbitrary initial condition given by a function of the position η ($F(\eta, 0) = F_0(\eta)$, $G(\eta, 0) = G_0(\eta)$, $H(\eta, 0) = H_0(\eta)$) is approximated by piecewise constant functions, by convenience, with equal width steps:

$$\begin{aligned} F &= \hat{F}_n(\eta) \approx F_{n_i} = \hat{F}_n(\eta_i + \theta_n \Delta\eta) \\ G &= \hat{G}_n(\eta) \approx G_{n_i} = \hat{G}_n(\eta_i + \theta_n \Delta\eta) \quad \text{for } \eta_i - \frac{\Delta\eta}{2} < \eta < \eta_i + \frac{\Delta\eta}{2} \\ H &= \hat{H}_n(\eta) \approx H_{n_i} = \hat{H}_n(\eta_i + \theta_n \Delta\eta) \end{aligned} \quad (4)$$

in which θ_n is a number randomly chosen in the open interval $(-1/2, +1/2)$ and $\Delta\eta$ is the width of each step ($\Delta\eta = \eta_{i+1} - \eta_i$). In the sequence, a Riemann problem – an initial value problem whose initial condition must be a step function – is to be solved for each two consecutive steps.

The above approximations for the initial data give rise, for each two consecutive steps, to the following Riemann problem – associated with equations (3)-(4):

$$\begin{aligned} \frac{\partial F}{\partial \tau} + \frac{\partial G}{\partial \eta} &= 0 \\ \frac{\partial G}{\partial \tau} + \frac{\partial}{\partial \eta} \left(\frac{G^2}{F} + \tilde{p}(F) \right) &= 0 \\ \frac{\partial H}{\partial \tau} + \frac{\partial}{\partial \eta} \left(\frac{GH}{F} \right) &= 0 \end{aligned} \quad (5)$$

with

$$\begin{aligned} (F, G, H) &= (F_{n_i}, G_{n_i}, H_{n_i}) \quad \text{for } \tau = \tau_n, \quad -\infty < \eta < \eta_i + \frac{\Delta\eta}{2} \\ (F, G, H) &= (F_{n_{i+1}}, G_{n_{i+1}}, H_{n_{i+1}}) \quad \text{for } \tau = \tau_n, \quad \eta_i + \frac{\Delta\eta}{2} < \eta < \infty. \end{aligned} \quad (6)$$

Denoting by \bar{F}_{n_i} , \bar{G}_{n_i} and \bar{H}_{n_i} the generalized solution of equations (5)-(6), the approximation for the solution of equations (3)-(4) at time τ_{n+1} is given as follows:

$$\begin{aligned} F &= \hat{F}_{n+1}(\eta) \approx \bar{F}_{n_i}(\eta, \tau_{n+1}) \\ G &= \hat{G}_{n+1}(\eta) \approx \bar{G}_{n_i}(\eta, \tau_{n+1}) \quad \text{for } \eta_i < \eta < \eta_{i+1} \\ H &= \hat{H}_{n+1}(\eta) \approx \bar{H}_{n_i}(\eta, \tau_{n+1}) \end{aligned} \quad (7)$$

Remark: In order to prevent interactions among nearby shocks of adjacent Riemann problems, the time step $\Delta\tau$ and, consequently, τ_{n+1} for problem (5)-(6), must be chosen in such a way that the Courant-Friedrichs-Lewy condition (Smoller, 1983) be satisfied, thus assuring the solution uniqueness:

$$\tau_{n+1} - \tau_n \leq \frac{\Delta\eta}{2|\lambda|_{\max}} \quad (8)$$

where $|\lambda|_{\max}$ is the maximum (in absolute value) propagation speed of shocks, considering all the Riemann problems at time τ_n .

4. The alternative procedure

The procedure proposed in this work consists in replacing the exact solution of the Riemann problem (5)-(6) by an approximation – built in by assuming any two given states always connected by a discontinuity which may not satisfy the entropy conditions – in order to advance in time through Glimm's scheme. Essentially the approximation consists in searching for a weak solution for the associated Riemann problem within a space of functions with a maximum of two jumps.

A generalized solution for the Riemann problem described in equations problems (5)-(6), depending on (η, τ) , may be expressed as a function of a similarity variable $\xi = \eta / \tau$ (Smoller, 1983; Saldanha da Gama, 1990) being constructed by connecting the left (L) and right (R) states to an intermediate state ($*$) by rarefactions or shocks as follows: $(F_L, G_L, H_L) \rightarrow (F_*, G_*, H_*) \rightarrow (F_R, G_R, H_R)$ or $(F_L, G_L) \rightarrow (F_*, G_*) \rightarrow (F_R, G_R)$.

A particular type of link is verified in problem (5)-(6) – the connection between intermediate states *1 and *2 is a contact shock (Lax, 1971; Smoller, 1983). In other words, the connection that would be called a 2-rarefaction – and would give rise to a continuous solution – cannot be found in problem (5)-(6), in which the second eigenvalue is coincident with the velocity that must be constant (Martins-Costa and Saldanha da Gama, 2003). This contact shock is characterized by absence of jump for both variables ρ and ρv – in such a way that $(\rho)_{*1} = (\rho)_{*2}$ and $(\rho v)_{*1} = (\rho v)_{*2}$. The jump is verified solely for $\rho \omega_A$, with a propagation speed v ($s_2 = \lambda_2 = v$) – the speed assuming the same value of the corresponding eigenvalue. A contact shock may be viewed as the limiting case of a rarefaction in which the rarefaction fan is reduced to a single line; namely a discontinuity with associated eigenvalue corresponding exactly to the shock speed (there is no entropy generation). Unlike ordinary shocks, the contact shock is reversible, without any associated entropy generation (Saldanha da Gama, 1990). So, the connections in the Riemann problem referred in equations (5)-(6) to be summarized as (Martins-Costa and Saldanha da Gama, 2003):

$$\begin{array}{ccccccc}
 L & \xRightarrow{R1 \text{ or } S1} & *1 & \xRightarrow{\text{Contact Shock}} & *2 & \xRightarrow{R3 \text{ or } S3} & R \\
 & & \omega_{A_1} = \omega_{A_L} & & \omega_{A_2} = \omega_{A_R} & & \\
 & & \rho_{*1} = \rho_{*2} = \rho_* & & & & \\
 & & v_{*1} = v_{*2} = v_* & & & &
 \end{array} \tag{9}$$

in which $R1$ and $R3$ denote possible rarefaction in connections 1 and 3 while $S1$ and $S3$ refer to possible shock in these connections. The result stated in equation (9) gives rise to an important simplification, allowing the former three-variables problem (5)-(6) to be reduced to a two variables (v and ρ) one with only two connections to be determined, namely, $L \xRightarrow{R1 \text{ or } S1} * \xRightarrow{R3 \text{ or } S3} R$. So, the referred states may be connected either by an i -rarefaction or an i -shock.

4.1. On the Riemann solver

The considerations above allow expressing the associated Riemann problem to system (5)-(6) as:

$$\left. \begin{array}{l} \frac{\partial F}{\partial \tau} + \frac{\partial G}{\partial \eta} = 0 \\ \frac{\partial G}{\partial \tau} + \frac{\partial}{\partial \eta} \left(\frac{G^2}{F} + p(F) \right) = 0 \end{array} \right\} \tau > \bar{\tau}, \quad -\infty < \eta < \infty \tag{10}$$

$$\begin{array}{ll} (F, G) = (F_L, G_R) & \text{for } \tau = \bar{\tau}, \quad \eta < \bar{\eta} \\ (F, G) = (F_R, G_R) & \text{for } \tau = \bar{\tau}, \quad \eta > \bar{\eta} \end{array} \tag{11}$$

The eigenvalues of (10) are given (in increasing order) by

$$\lambda_i = \frac{G}{F} + (-1)^i (p')^{1/2} = v + (-1)^i (p')^{1/2} \quad i = 1, 2 \tag{12}$$

Since $p' > 0$ for all η and τ , (10)-(11) is a hyperbolic system (genuinely nonlinear provided p'' is positive (or negative) everywhere). Problem (10)-(11) is called a Riemann problem whose generalized solution depends on the ratio $(\eta - \bar{\eta}) / (\tau - \bar{\tau})$, being reached by connecting the left state (F_L, G_L) and the right state (F_R, G_R) to an intermediate state (F_*, G_*) , as stated before $L \xRightarrow{\text{Raref or Shock}} * \xRightarrow{\text{Raref or Shock}} R$.

Two states are connected by an i -rarefaction (Lax, 1971; John, 1974) – a continuous solution of the associated Riemann problem – when the corresponding eigenvalues λ_i are increasing functions of $(\eta - \bar{\eta}) / (\tau - \bar{\tau})$ between these states. In this case the solution (F, G) depends continuously on $(\eta - \bar{\eta}) / (\tau - \bar{\tau})$ between these two states and associated to an i -rarefaction there exists a Riemann invariant given by:

$$R_i = v - (-1)^i \int \frac{\sqrt{p}}{\rho} d\rho = \text{constant} \quad i = 1, 2 \quad (13)$$

This invariant is a constant between two states connected by an i -rarefaction.

If the eigenvalues λ_i are decreasing functions of $(\eta - \bar{\eta})/(\tau - \bar{\tau})$, the states are connected by an i -shock (a discontinuous solution) with speed s_i and the entropy conditions are automatically satisfied. Since weak solutions cannot assure uniqueness of solution (Keyfitz and Kranzer, 1978), the so-called entropy condition must be verified in order that uniqueness is preserved. Considering two given states connected by an i -Shock with speed s_i , the following jump conditions – denoted as Rankine-Hugoniot conditions – associated with equation (10), must be satisfied:

$$s_i = \frac{[[G]]}{[[F]]} = \frac{[[G^2 / F + p]]}{[[G]]} \quad (14)$$

in which s_i represents the speed of discontinuity propagation and $[[f]]$, the jump of a quantity f .

The main purpose of the present work is the proposition of a Riemann solver, which consists of assuming the solution within a space of piecewise constant functions. So that any two given states will be connected by a shock. In other words

$$(F_L, G_L) \rightarrow \text{1-shock} \rightarrow (F_*, G_*) \rightarrow \text{2-shock} \rightarrow (F_R, G_R) \quad (15)$$

This approximation no longer requires considering the original four possible solutions: $(F_L, G_L) \xrightarrow[\text{Raref or Shock}]{} (F_*, G_*) \xrightarrow[\text{Raref or Shock}]{} (F_R, G_R)$. On the other hand, the entropy conditions are not ensured. It is to be noticed that the conservation laws are satisfied in a weak sense.

The (generalized) solution of (10)-(11), within a space of piecewise constant functions, is reached as follows ($z = (\eta - \bar{\eta})/(\tau - \bar{\tau})$)

$$(F, G) = \begin{cases} (F_L, G_L) & \text{if } -\infty < z < s_1 \\ (F_*, G_*) & \text{if } s_1 < z < s_2 \\ (F_R, G_R) & \text{if } s_2 < z < \infty \end{cases} \quad (16)$$

For instance, when $p = \rho^2$, we have

$$\begin{aligned} v_* - v_L &= -(\rho_* - \rho_L) \left[\left(\frac{p_* - p_L}{\rho_* - \rho_L} \right) \frac{1}{\rho_* \rho_L} \right]^{1/2} \\ v_R - v_* &= (\rho_R - \rho_*) \left[\left(\frac{p_R - p_*}{\rho_R - \rho_*} \right) \frac{1}{\rho_R \rho_*} \right]^{1/2} \end{aligned} \quad (17)$$

being ρ_* the unique positive root (always exists) of

$$v_R - v_L = (\rho_R - \rho_*) \left[\left(\frac{p_R - p_*}{\rho_R - \rho_*} \right) \frac{1}{\rho_R \rho_*} \right]^{1/2} - (\rho_* - \rho_L) \left[\left(\frac{p_* - p_L}{\rho_* - \rho_L} \right) \frac{1}{\rho_* \rho_L} \right]^{1/2} \quad (18)$$

while the shock speeds are given by

$$s_1 = \frac{G_* - G_L}{F_* - F_L} = \frac{\rho_* v_* - \rho_L v_L}{\rho_* - \rho_L} \quad \text{and} \quad s_2 = \frac{G_R - G_*}{F_R - F_*} = \frac{\rho_R v_R - \rho_* v_*}{\rho_R - \rho_*} \quad (19)$$

It is convenient to evaluate v_* from

$$v_* - v_L = \frac{1}{2} \left\{ -(\rho_* - \rho_L) \left[\left(\frac{p_* - p_L}{\rho_* - \rho_L} \right) \frac{1}{\rho_* \rho_L} \right]^{1/2} - (\rho_R - \rho_*) \left[\left(\frac{p_R - p_*}{\rho_R - \rho_*} \right) \frac{1}{\rho_R \rho_*} \right]^{1/2} \right\} + \frac{v_L + v_R}{2} \quad (20)$$

In all the above stated solutions the quantities λ and s are such that

$$\begin{aligned} \lambda_{1_L} &= (G/F)_L - \sqrt{(\tilde{p}')_L} & \text{with } (\tilde{p}')_L &= \frac{d\tilde{p}}{dF} \Big|_{F=F_L} \\ \lambda_{1_*} &= (G/F)_* - \sqrt{(\tilde{p}')_*} & \text{with } (\tilde{p}')_* &= \frac{d\tilde{p}}{dF} \Big|_{F=F_*} \\ \lambda_{3_*} &= (G/F)_* + \sqrt{(\tilde{p}')_*} & \text{with } (\tilde{p}')_* &= \frac{d\tilde{p}}{dF} \Big|_{F=F_*} \\ \lambda_{3_R} &= (G/F)_R + \sqrt{(\tilde{p}')_R} & \text{with } (\tilde{p}')_R &= \frac{d\tilde{p}}{dF} \Big|_{F=F_R} \end{aligned} \quad (21)$$

and

$$s_1 = \frac{G_L - G_*}{F_L - F_*} \quad s_2 = (G/F)_* \quad s_3 = \frac{G_* - G_R}{F_* - F_R} \quad (22)$$

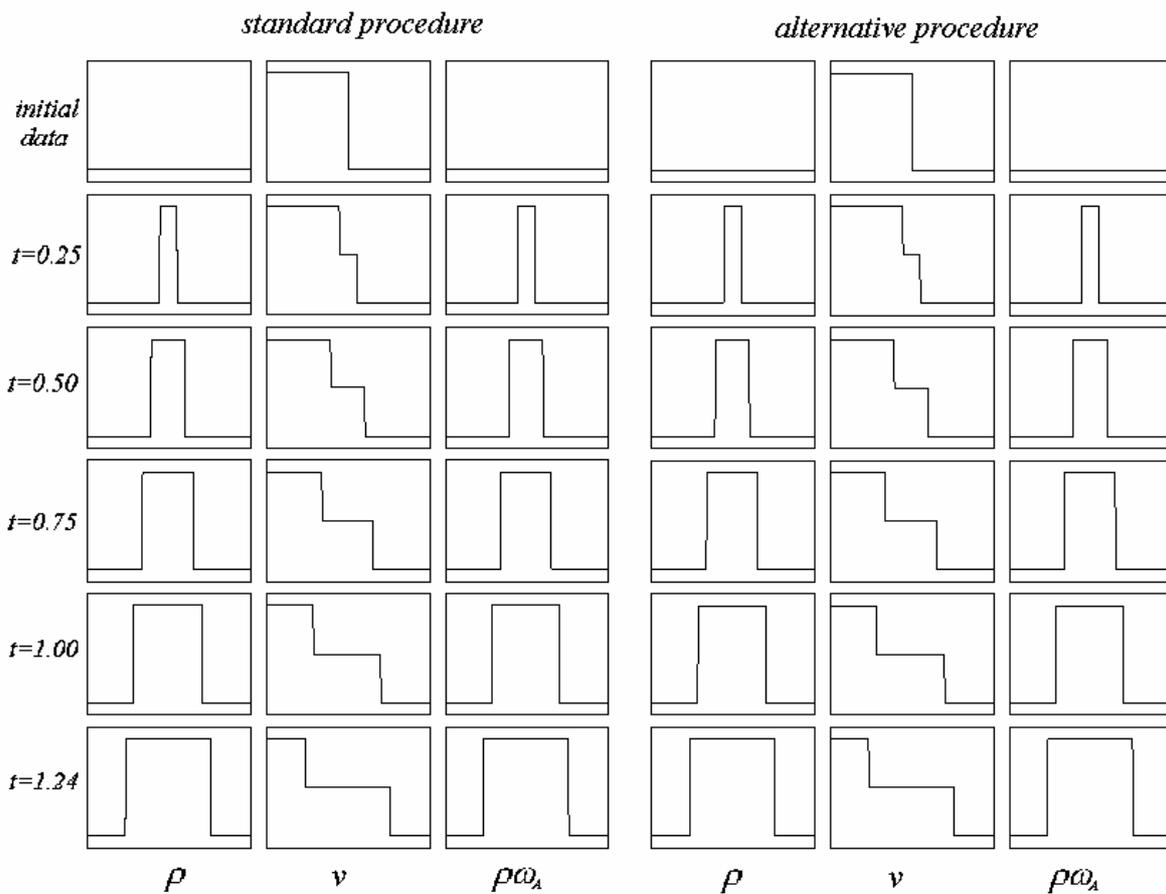


Figure 1. Gas density, velocity and pollutant concentration per unit volume variation with position - Left: Riemann exact solution; Right: Riemann solver. Initial data: constant ρ and ω_A and step function for v .

5. Some results

Figures 1 to 4 show results for gas density, velocity and pollutant concentration per unit volume for five selected time instants, allowing to observe the good performance of the Riemann solver presented in this work. In all the depicted results the vertical axis corresponds to the numerical value assumed by one of these three considered variables, the horizontal one being the spatial coordinate x . Besides, all the qualitative results exhibited were obtained by employing a convenient normalization, in such a way that zero and unit displayed values for the variables associated with ρ , v and $\rho\omega_A$ correspond to the minimum and maximum actual values in which ρ , v and $\rho\omega_A$ are redefined as:

$$\frac{\rho - (\rho)_{\min}}{(\rho)_{\max} - (\rho)_{\min}} \rightarrow \rho \quad \frac{v - (v)_{\min}}{(v)_{\max} - (v)_{\min}} \rightarrow v \quad \frac{\rho\omega_A - (\rho\omega_A)_{\min}}{(\rho\omega_A)_{\max} - (\rho\omega_A)_{\min}} \rightarrow \rho\omega_A.. \quad (23)$$

It is important to notice that neither ρ nor ω_A assume negative values. In all the results an unbounded domain $(-\infty < x < \infty)$ is considered with distinct initial data to show the evolution of gas density, velocity and pollutant concentration per unit volume.

The three columns at the left hand side – namely a set composed by three columns and six lines, each line representing a distinct time instant, the first one being the imposed initial condition – depict ρ , v and $\rho\omega_A$ obtained by employing Glimm’s scheme with 300 steps for each time advance built from the exact solution of the associated Riemann problem. The three columns at the right hand side show equivalent results for ρ , v and $\rho\omega_A$ also obtained by using Glimm’s scheme with 300 steps for each advance in time but constructed by using the Riemann solver proposed in this work.

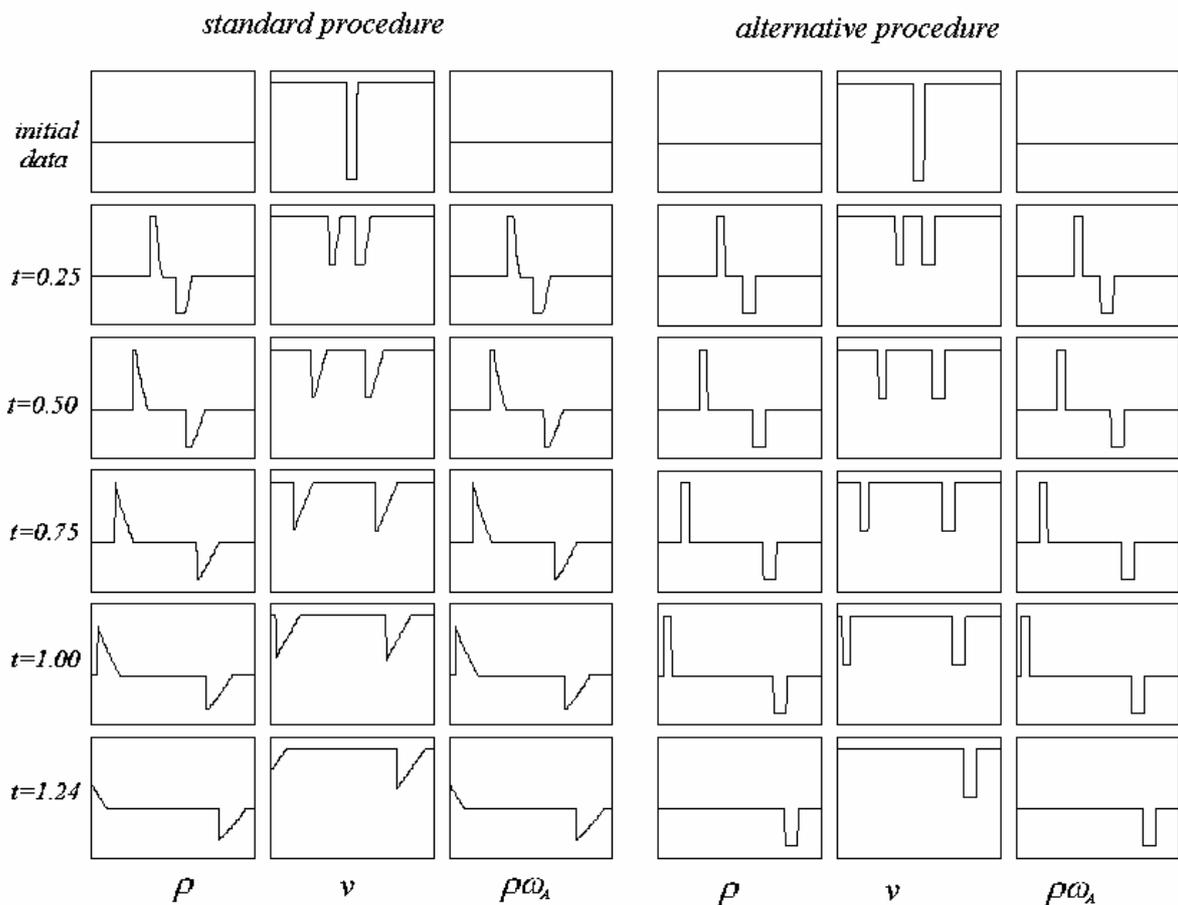


Figure 2. Gas density, velocity and pollutant concentration per unit volume variation with position - Left: Riemann exact solution; Right: Riemann solver. Initial data: constant ρ and ω_A and a small low velocity region for v .

In Fig. 1 the initial data consist of a shock prescribed for the velocity while constant values are prescribed for both the mass density and the concentration of the constituent A (pollutant) in the mixture. Since the results obtained through the exact solution of Riemann problem – depicted at the first three columns – give rise essentially to connections by shocks, the Riemann solver presented in this work (depicted at the three last columns) shows a very good agreement with those obtained by employing the exact solution. It is important to mention that a relatively small number of time steps (namely 300) was employed for all the considered cases, resulting in a very rapid convergence in both cases.

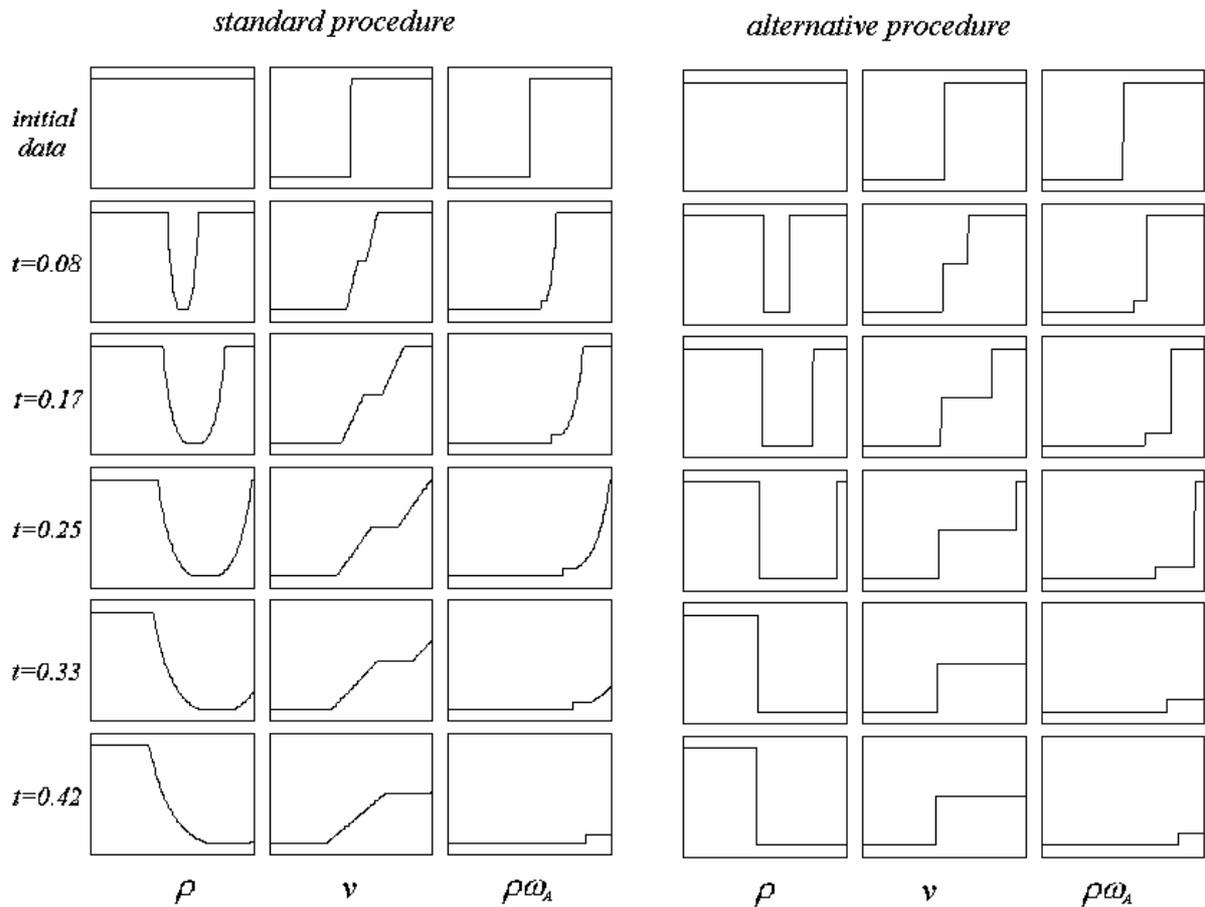


Figure 3. Gas density, velocity and pollutant concentration per unit volume variation with position - Left: Riemann exact solution; Right: Riemann solver. Initial data: constant ρ and distinct step functions for v and ω_A , being $v_L > v_R$ and $\omega_{AL} < \omega_{AR}$

Figure 2 has been obtained by considering as initial data a constant (unit) value for the mass density ρ and a constant value for the pollutant concentration ($\omega_A = 0.5$). A very small low velocity region (with $v = -1.0$) was imposed near the center of the depicted domain, while outside this region a higher value ($v = 0$) has been considered. Comparing the results obtained through Riemann problem exact solution to those using the alternative procedure proposed in this work, a good agreement may be noticed, the shocks being at the same spatial position in both cases, although the proposed Riemann solver is – as expected – unable to capture exactly the connections by rarefactions obtained in the exact solution.

Figure 3 has been obtained by considering as initial data a constant (unit) value for the mass density ρ , step functions for the velocity – placed near the center of the depicted domain, being $v_L > v_R$ and another step function for ω_A , with $\omega_{AL} < \omega_{AR}$, its jump absolute value being ten times smaller than the velocity one. A tendency to present a very low density region – which size increases with time – may be detected by observing Figure 3. Comparing the results obtained by the standard (exact) procedure with those obtained through the proposed Riemann solver, although

the shocks are at the same spatial position in both cases, the alternative procedure was unable to capture the smooth connections presented when the exact solution is used, due to this Riemann solver philosophy which consists in substituting both continuous and discontinuous solutions by shocks.

It is worth mentioning that the three columns at the left hand side of figures 2 and 3 have already been presented in Martins-Costa and Saldanha da Gama (2003), in which they are compared aiming at analyzing the influence of discontinuities imposed on the velocity field in an infinite domain.

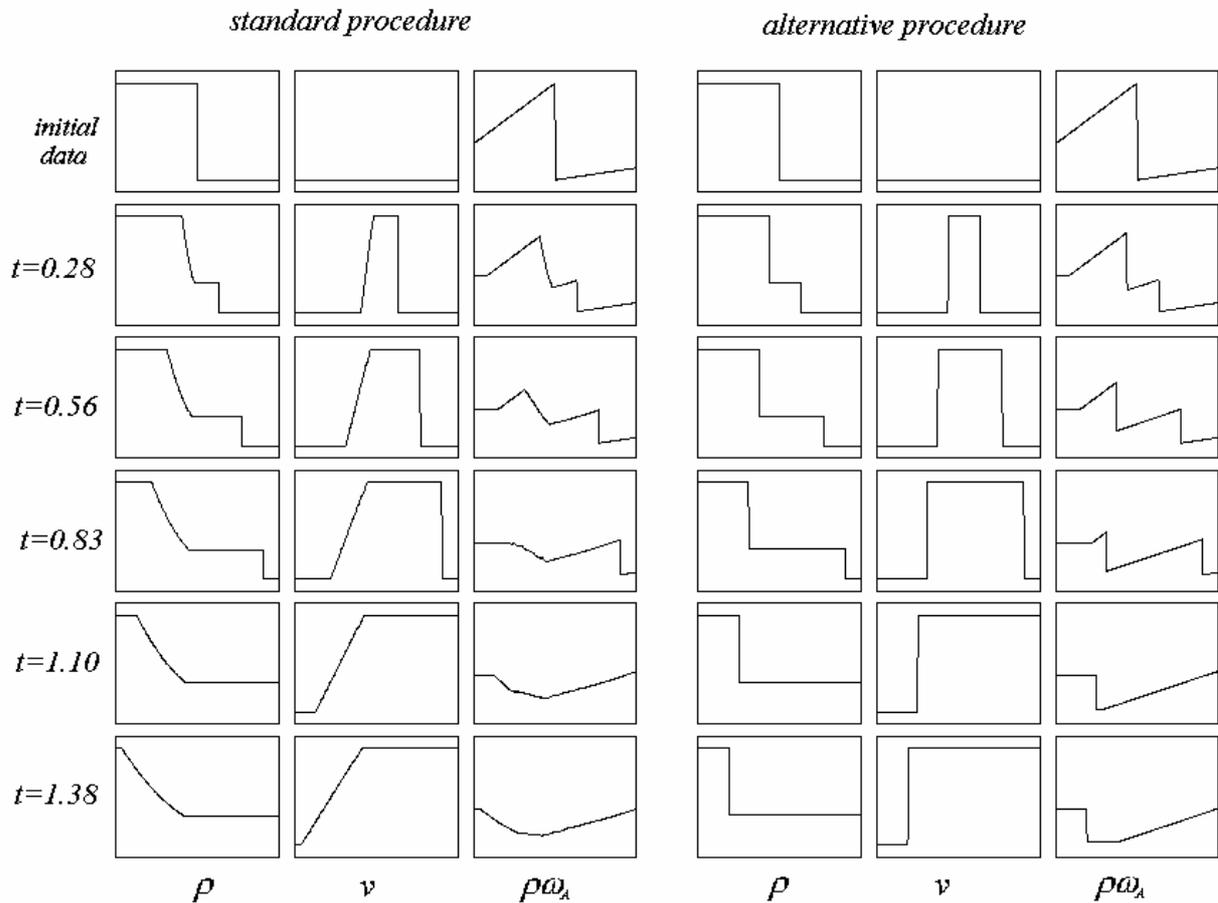


Figure 4. Gas density, velocity and pollutant concentration per unit volume variation with position - Left: Riemann exact solution; Right: Riemann solver. Initial data: zero v and step function for ρ and a discontinuous ω_A with two distinct linear functions.

Figure 4 shows results for gas density, velocity and pollutant concentration per unit volume variation with position considering both the exact and the approximate solution for the associated Riemann problem and initial conditions given by zero v and step function for ρ and a discontinuous ω_A with two decreasing linear functions with distinct inclination. As expected, all the connections by shocks obtained through the exact solution are preserved at their exact position by employing the Riemann solver.

6. Final remarks

Glimm's method is a convenient tool for solving nonlinear hyperbolic problems, exhibiting features such as low storage costs (no matrix storage is required – only 10 vectors with 300 positions have been used) and low computational effort (circa 2 minutes CPU time in a Pentium IV, 2.4 GHz, 128 Mb RAM), when compared to other numerical procedures to approximate nonlinear problems.

Regarding its accuracy, the method is free from numerical dissipation – preserving shock waves magnitude and presenting a deviation from the correct position smaller than the width of each step – preserving shock waves position. Besides, if the width of the steps tends to zero, Glimm's approximation tends to the exact solution of the problem. However, two important shortcomings of this methodology must be mentioned: the former its applicability being restricted to one-dimensional problems and the latter its implementation requiring previous knowledge of a solution of the associated Riemann problem – usually not an easy task.

The numerical methodology presented in this work allowed the good approximation of a nonlinear system of three partial differential equations representing mathematically the transport of a pollutant in the atmosphere. Additional effects not considered in this work such as diffusion of the pollutant in the atmosphere, generation of the pollutant (by chemical reactions, for instance) as well as gravitational effects could be accounted for by employing an operator splitting technique (see Martins-Costa and Saldanha da Gama, 2001 and references therein).

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8. References

- Chorin AJ, 1976, Random choice solution of hyperbolic systems. *J. Comput. Physics*. Vol. 22, pp. 517-533.
- Glimm J., 1965, Solutions in the large for nonlinear hyperbolic systems of equations. *Comm. Pure Appl. Math.* Vol. 18 pp. 697-715.
- John F., 1974, Formation of singularities in onedimensional nonlinear wave propagation. *Comm. Pure Appl. Math.* Vol. 27, pp. 337-405.
- John F., 1982, *Partial Differential Equations*. Berlin, Springer-Verlag.
- Keyfitz, B., Kranzer, H., 1978, Existence and uniqueness of entropy solutions to the Riemann problem for hyperbolic systems of two nonlinear conservation laws. *J. Diff. Eqns.* Vol. 27, pp. 444-476.
- Lax, P., 1971, *Shock Waves and Entropy*, in *Contributions to Nonlinear Functional Analysis*. New York: Academic Press.
- Martins-Costa, M.L. and Saldanha da Gama, R.M., 2003, "Glimm's Method Simulation for the Pollutant Transport in an Isothermal Atmosphere", *Comput. Mech.*, Vol. 32, No. 3, pp. 214-223.
- Saldanha da Gama, R.M., 1990, An Alternative Procedure for Simulating the Dynamical Response of Non-Linear Elastic Rods, *Int. J. Num. Meth. Engng.*, Vol. 29, pp. 123-139.
- Smoller J., 1983, *Shock-Waves and Reaction-Diffusion Equations*. Berlin, Springer-Verlag.

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