

# Flux vector splitting and stationary contact discontinuity

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## Abstract

In order to capture in a stable and accurate way a boundary layer with an upwind finite volume scheme, numerical analysis of stationary contact discontinuity problem shows that a flux vector splitting generates in general a numerical viscosity proportional to the difference of densities whereas numerical viscosity is null for a flux difference splitting approximating all the waves of a Riemann problem.

## Résumé

Pour capturer de façon précise et stable une couche limite avec un schéma de volumes finis, l'analyse numérique du problème de la discontinuité de contact stationnaire montre qu'une décomposition de flux génère en général une viscosité numérique proportionnelle à la différence de densité alors qu'il n'en est rien avec une résolution approchée du problème de Riemann.

## Plan

- 1) Introduction
- 2) Left-right invariance
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### 1) Introduction.

• We study the Euler equations of gas dynamics in one space dimension. They take the form of an hyperbolic system of conservation laws between state  $W$  and physical flux  $f(W)$  :

$$(1.1) \quad \frac{\partial W}{\partial t} + \frac{\partial}{\partial x} f(W) = 0$$

where state  $W = W(t, x) \in \mathbb{R}^3$  represents a volumic density of mass, momentum and energy :

$$(1.2) \quad W = (\rho, \rho u, \rho E \equiv \rho e + \frac{1}{2}\rho u^2)^t.$$

Algebraic form of physical flux  $f(W) \in \mathbb{R}^3$  is given by

$$(1.3) \quad f(W) = (\rho u, \rho u^2 + p, \rho u E + pu)^t;$$

it uses pressure, which is a function of density  $\rho$  and of internal energy  $e$  parameterized for a polytropic perfect gas by ratio  $\gamma > 1$  of specific heats :

$$(1.4) \quad p = (\gamma - 1) \rho e.$$

• In order to approach numerically solutions of system (1.1), we introduce the so-called finite volume method ; space is discretized with a grid  $j \Delta x$  ( $j \in \mathbb{Z}$ ) and time by multiples  $n \Delta t$  ( $n \in \mathbb{N}$ ) of time step  $\Delta t$ . We search an approximate value  $W_j^n$  of field  $W(\bullet, \bullet)$  at particular vertex  $j \Delta x$  and discrete time level  $n \Delta t$  thanks to the family of numerical fluxes  $f_{j+1/2}^{n+1/2}$  ( $j \in \mathbb{Z}$ ,  $n \in \mathbb{N}$ ) (see e.g. Harten, Lax and Van Leer [HLV83]) :

$$(1.5) \quad \frac{1}{\Delta t} (W_j^{n+1} - W_j^n) + \frac{1}{\Delta x} (f_{j+1/2}^{n+1/2} - f_{j-1/2}^{n+1/2}) = 0.$$

In this communication, we restrict ourselves to a two-point numerical flux function that is explicit and first order accurate in space and time, e.g. of the form :

$$(1.6) \quad f_{j+1/2}^{n+1/2} = \Phi(W_j^n, W_{j+1}^n).$$

• We distinguish between two types of numerical flux functions depending of two arguments : on one side, exact or approximate solutions of the Riemann problem ("flux difference splitting") between states  $W_j^n$  and  $W_{j+1}^n$  (see e.g. Godlewski-Raviart [GR96] for mathematical and numerical context) with numerical fluxes proposed by Godunov [Go59], Roe [Roe81] and Osher [Os81] and on the other side flux decompositions ("flux vector splitting"). A flux vector splitting, with Sanders-Prendergast [SP74], Steger-Warming [SW81], Van Leer [VL82], Bourdel, Delorme and Mazet [BDM89] or Perthame [Pe91]

among others, suppose that the physical flux function  $\mathbb{R}^3 \ni W \longmapsto f(W) \in \mathbb{R}^3$  explicited in (1.3) has been written under the form

$$(1.7) \quad f(W) = f^+(W) + f^-(W)$$

with a set of constraints on functions  $f^+(\bullet)$  and  $f^-(\bullet)$  detailed for example in the book of Godlewski and Raviart [GR96]. For modelling upwinding, the numerical flux admits the following very simple form :

$$(1.8) \quad \Phi(W_l, W_r) = f^+(W_l) + f^-(W_r).$$

- In the context of a stationary aerodynamics problem, Van Leer, Thomas, Roe and Newsome [VTRN87] compare Van Leer flux vector splitting [VL82] and Roe scheme [Roe81] that uses a Riemann problem for a linearized equation. They show that in order to give a correct prediction of skin friction coefficient and heat flux on the boundary of a moving body with a numerical approximation of the Navier-Stokes equations of gas dynamics, it is not possible to use Van Leer flux vector splitting of the type (1.8) for convective part of fluid flow. Their conclusion is to reject flux vector splitting methodology if the objective is to predict more than the simple pressure field.

- In fact, the problem occurs in the boundary layer. Along the direction  $x$  normal to the boundary, normal velocity  $u$  is very small. Then it is natural to study the evolution of a flux vector splitting (1.8) for the very simple model of a stationary contact discontinuity, i.e. a boundary layer with infinitesimal thickness. It is a particular problem of decomposition of discontinuity where given states  $W_l$  and  $W_r$  define on one hand a velocity field identically null composed by  $u_l$  for  $x < 0$  and by  $u_r$  for  $x > 0$  :

$$(1.9) \quad u_l = u_r = 0,$$

and on the other hand a pressure field denoted respectively by  $p_l$  for  $x < 0$  and  $p_r$  for  $x > 0$  without discontinuity :

$$(1.10) \quad p_l = p_r = p.$$

Physical solution of such a stationary contact discontinuity does not depend on time : density jump is maintained at the interface  $x = 0$  as long as time is increasing and it is the addition of viscous term or of geometrical perturbations like in Kelvin-Helmholtz instability that modify the interface, which is crucial for a correct capture of boundary layers and shear instabilities.

- In this note, we prove that in a general way if a flux vector splitting satisfies very natural hypotheses of left-right invariance (section 2), then the associated scheme for gas dynamics contains a numerical viscosity essentially proportional to the jump of density, then of the order zero relatively to space step (section 3).

## 2) Left-right invariance.

• We consider transformation  $\sigma$  of state  $W$  obtained by changing the sign of velocity :

$$(2.1) \quad \sigma \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} = \begin{pmatrix} \rho \\ -\rho u \\ \rho E \end{pmatrix} .$$

Taking into account relations (1.2) and (1.3), we observe that

$$(2.2) \quad f(\sigma W) + \sigma f(W) = 0;$$

when we change the sign of velocity, we change the sign of mass flux and of energy flux but we do not the sign of momentum flux.

• Because changing the sign of velocity is equivalent to changing the sign of space direction  $x$ , it is useful to introduce the normal unitary vector  $n$  to this direction ( $n \in \{-1, 1\}$ ) and to set

$$(2.3) \quad g(n, W) = \begin{pmatrix} \rho(u \cdot n) \\ (\rho u^2 + p)n \\ (\rho E + p)(u \cdot n) \end{pmatrix}$$

and also

$$(2.4) \quad \sigma n = -n .$$

If we change both signs of velocity and of space direction, mass and energy fluxes remain unchanged but sign of momentum flux is changed. We have in consequence :

$$(2.5) \quad g(\sigma n, \sigma W) = \sigma g(n, W) .$$

• Natural extension of this left-right invariance property to the numerical flux can be formalized by setting :

$$(2.6) \quad \Psi(W_l, n, W_r) = \begin{cases} \Phi(W_l, W_r) & \text{if } n = +1 \\ -\Phi(W_l, W_r) & \text{if } n = -1 . \end{cases}$$

The left-right invariance for numerical flux consists to say that if we exchange both left and right states, the sign of their velocity and the normal direction, we only change the sign of momentum flux in an algebraic relation analogous to (2.2).

**Definition 1. Left-right invariance property.**

The numerical flux function  $(W_l, W_r) \mapsto \Phi(W_l, W_r)$  satisfies the left-right invariance property if the function  $\Psi(\bullet, \bullet, \bullet)$  defined in (2.6) and operator  $\sigma$  defined at relations (2.1) and (2.4) satisfy the condition

$$(2.7) \quad \Psi(\sigma W_r, \sigma n, \sigma W_l) - \sigma \Psi(W_l, n, W_r) = 0 .$$

- We remark that consistency condition

$$(2.8) \quad \Phi(W, W) = f(W)$$

can be translated for the pair  $(\Psi, g)$  by the relation

$$(2.9) \quad \Psi(W, n, W) = g(n, W)$$

and in this particular case, relation (2.5) shows that

$$\Psi(\sigma W, \sigma n, \sigma W) - \sigma \Psi(W, n, W) = g(\sigma n, \sigma W) - \sigma g(n, W) = 0.$$

This remark establishes a particular case of relation (2.7) when  $W_l = W_r = W$ .

**Proposition 1. Left-right invariance of a flux vector splitting.**

A flux vector splitting (1.7) associated with a numerical flux function (1.8) satisfies the left-right invariance property if and only if we have

$$(2.10) \quad f^+(\sigma W) + \sigma f^-(W) = 0 \quad \forall W$$

which means

$$(2.11) \quad f_j^+(\sigma W) = -f_j^-(W), \quad j = 1 \text{ and } j = 3$$

$$(2.12) \quad f_2^+(\sigma W) = f_2^-(W).$$

**Proof of Proposition 1.**

- We introduce representation (1.8) inside relation (2.7) when  $n = +1$  :

$$\begin{aligned} & \Psi(\sigma W_r, \sigma n, \sigma W_l) - \sigma \Psi(W_l, n, W_r) = \\ & = -\Phi(\sigma W_r, \sigma W_l) - \sigma \Phi(W_l, W_r) \\ & = -[f^+(\sigma W_r) + f^-(\sigma W_l)] - \sigma [f^+(W_l) + f^-(W_r)] \\ & = -[f^+(\sigma W_r) + \sigma f^-(W_r)] - \sigma [f^+(W_l) + \sigma f^-(\sigma W_l)] \\ & \qquad \qquad \qquad \text{because } \sigma^2 = \text{Id} \\ & = 0 \qquad \qquad \text{for each pair } (W_l, W_r). \end{aligned}$$

If we make the choice of two independent states  $W_l$  and  $W_r$  the preceding relation states clearly relation (2.10) and when we explicit the action of operator  $\sigma$  on a vector (see relation (2.1)), we obtain the detail of the algebra for each component, i.e. relations (2.11) and (2.12).

- On the other way, if condition (2.10) is satisfied, then relation (2.7) is correct for  $n = 1$  ; it remains true for  $n = -1$  because the left member is an odd function of variable  $n$  due to relation (2.6). In consequence the proposition is established. □

**Proposition 2. Particular case of classical flux vector splittings.**

Van Leer flux, Sanders Prendergast flux and Boltzmann schemes satisfy the left-right invariance property.

**Proof of Proposition 2.**

- Van Leer flux satisfy the following relation

$$(2.13) \quad f^+(W) = f(W) \quad \text{if } M \equiv \frac{u}{c} \geq 1$$

$$(2.14) \quad f^-(W) = f(W) \quad \text{if } M \leq -1.$$

If the Mach number  $M$  of state  $W$  is greater or equal to 1, then the Mach number of state  $\sigma W$  is lower or equal to  $-1$ ; then  $f^+(\sigma W) = 0 = -\sigma f^-(W)$  and relation (2.10) is established in this case. If on the contrary  $M \leq -1$ , then  $f^+(\sigma W) = f(\sigma W)$  and  $f^-(W) = f(W)$  and relation (2.10) is in this case a simple re-writing of relation (2.2).

- When  $|M| \leq 1$ , Van Leer flux vector splitting satisfies the relation

$$(2.15) \quad f^+(W) = \begin{pmatrix} \rho c \left(\frac{M+1}{2}\right)^2 \\ \rho c \left(\frac{M+1}{2}\right)^2 \frac{(\gamma-1)u + 2c}{\gamma} \\ \rho c \left(\frac{M+1}{2}\right)^2 \frac{((\gamma-1)u + 2c)^2}{2(\gamma^2-1)} \end{pmatrix}$$

$$(2.16) \quad f^-(W) = \begin{pmatrix} -\rho c \left(\frac{M-1}{2}\right)^2 \\ -\rho c \left(\frac{M-1}{2}\right)^2 \frac{(\gamma-1)u - 2c}{\gamma} \\ -\rho c \left(\frac{M-1}{2}\right)^2 \frac{((\gamma-1)u - 2c)^2}{2(\gamma^2-1)} \end{pmatrix}.$$

Relation (2.10) is clear. Consistency condition (1.7) is not obvious; the proof is an algebraic calculus introduced in the original work [VL82].

- In the case of a Boltzmann scheme, we write state  $W$  under the particular form

$$(2.17) \quad W = \int_{-\infty}^{+\infty} \chi\left(\frac{|v-u|}{\sqrt{T}}\right) \left(1, v, \frac{1}{2}|v|^2\right)^t dv$$

where  $\chi(\bullet)$  is a positive function that defines the numerical scheme and  $T$  is the temperature. The flux is simply evaluated by

$$(2.18) \quad f(W) = \int_{-\infty}^{+\infty} \chi\left(\frac{|v-u|}{\sqrt{T}}\right) \left(v, |v|^2, \frac{v}{2}|v|^2\right)^t dv.$$

To take into account the fact that flux  $f^+$  represents the action of all the particles going from left to right, we set

$$(2.19) \quad f^+(W) = \int_0^{+\infty} \chi\left(\frac{|v-u|}{\sqrt{T}}\right) (v, |v|^2, \frac{v}{2} |v|^2)^t dv$$

and in an analogous way, due to (1.7) :

$$(2.20) \quad f^-(W) = \int_{-\infty}^0 \chi\left(\frac{|v-u|}{\sqrt{T}}\right) (v, |v|^2, \frac{v}{2} |v|^2)^t dv.$$

After having made the change of variable  $v \mapsto -v$  inside the integral (2.19), we deduce

$$(2.21) \quad f^+(\sigma W) = \int_{-\infty}^0 \chi\left(\frac{|v-u|}{\sqrt{T}}\right) (-v, |v|^2, -\frac{v}{2} |v|^2)^t dv$$

and relation (2.10) est clear.

• We consider now the case of Sanders and Prendergast splitting ; we just replace function  $\chi$  of relation (2.19) by a linear combination of Dirac measures at particular points  $u-c, u, u+c$  in velocity space, where  $c$  is the sound waves celerity, in order to satisfy the following relations

$$(2.22) \quad \rho = \int_{-\infty}^{+\infty} d\mu(v)$$

$$(2.23) \quad \rho u = \int_{-\infty}^{+\infty} v d\mu(v)$$

$$(2.24) \quad \rho u^2 + p = \int_{-\infty}^{+\infty} v^2 d\mu(v).$$

Then total energy  $\rho E$  is decomposed under the form

$$(2.25) \quad \rho E = \frac{1}{2} \int_{-\infty}^{+\infty} v^2 d\mu(v) + \left(e - \frac{p}{2\rho}\right) \int_{-\infty}^{+\infty} d\mu(v)$$

and the particular algebraic form that controls the measure  $d\mu(v)$  [SP74] allows to deduce

$$(2.26) \quad \rho u E + pu = \frac{1}{2} \int_{-\infty}^{+\infty} v^3 d\mu(v) + \left(e - \frac{p}{2\rho}\right) \int_{-\infty}^{+\infty} v d\mu(v).$$

In an way analogous to the other Boltzmann schemes, the flux vector splitting results from an integration on the interval  $]0, +\infty[$  to evaluate  $f^+$  and on the opposite interval  $] -\infty, 0[$  for  $f^-$ . Even parity of  $f_2^\pm$  is a consequence of parity of relation (2.24) whereas odd parity of  $f_1^\pm$  and  $f_3^\pm$  is a consequence of imparity of relations (2.23) and (2.26). This result establishes relation (2.10) for Boltzmann schemes and Proposition 2 is proven.  $\square$

### 3) Numerical viscosity on a stationary contact.

**Definition 2. Numerical viscosity.**

Numerical viscosity  $V(W_l, W_r)$  of a two-point numerical scheme of the type (1.6) is defined by the relation

$$(3.1) \quad \Phi(W_l, W_r) = \frac{1}{2}(f(W_l) + f(W_r)) - \frac{1}{2}V(W_l, W_r).$$

**Proposition 3. Numerical viscosity of a flux vector splitting.**

Let  $\Phi(\bullet, \bullet)$  be a flux vector splitting of the type (1.8). Then numerical viscosity  $V(W_l, W_r)$  satisfies the relation

$$(3.2) \quad V(W_l, W_r) = (f^+(W_r) - f^-(W_r)) - (f^+(W_l) - f^-(W_l)).$$

**Proof of Proposition 3.**

• It results from the following calculus :

$$\begin{aligned} V(W_l, W_r) &= f(W_l) + f(W_r) - 2\Phi(W_l, W_r) && \text{due to (3.1)} \\ &= (f^+(W_l) + f^-(W_l)) + (f^+(W_r) + f^-(W_r)) - 2(f^+(W_l) + f^-(W_r)) \\ &&& \text{due to (1.6) and (1.7)} \\ &= (f^+(W_r) - f^-(W_r)) - (f^+(W_l) - f^-(W_l)) \end{aligned}$$

and relation (3.2) is established.  $\square$

**Proposition 4. Stationary contact discontinuity.**

Let  $W$  be a state with a velocity equal to zero. It satisfies in particular

$$(3.3) \quad \sigma W = W.$$

Then if flux vector splitting  $\Phi(\bullet, \bullet)$  defined in (1.7)-(1.8) satisfies the left-right invariance property, there exists two functions  $]0, +\infty[^2 \ni (\rho, p) \mapsto \mu(\rho, p) \in \mathbb{R}$  and  $]0, +\infty[^2 \ni (\rho, p) \mapsto \epsilon(\rho, p) \in \mathbb{R}$  in order to satisfy

$$(3.4) \quad f^+(W) = \frac{1}{2} \begin{pmatrix} \mu(\rho, p) \\ p \\ \epsilon(\rho, p) \end{pmatrix} \quad \text{if } \sigma W = W$$

$$(3.5) \quad f^-(W) = \frac{1}{2} \begin{pmatrix} -\mu(\rho, p) \\ p \\ -\epsilon(\rho, p) \end{pmatrix} \quad \text{if } \sigma W = W.$$

Moreover, for a stationary contact discontinuity (1.9)-(1.10), numerical viscosity satisfies

$$(3.6) \quad V(W_l, W_r) = \begin{pmatrix} \mu(\rho_r, p) - \mu(\rho_l, p) \\ 0 \\ \epsilon(\rho_r, p) - \epsilon(\rho_l, p) \end{pmatrix}.$$

• In the case of Van Leer flux vector splitting, relations (2.15) and (2.16) show

$$(3.7) \quad \mu^{VL}(\rho, p) = \frac{1}{2}\sqrt{\gamma\rho p}$$



$$(3.8) \quad \epsilon^{VL}(\rho, p) = \frac{\gamma\sqrt{\gamma}}{\gamma^2 - 1} \frac{p\sqrt{p}}{\sqrt{\rho}}$$

and for a Boltzmann scheme, we have, taking into account (2.19) and (2.20),

$$(3.9) \quad \mu^B(\rho, p) = 2 \int_0^{+\infty} \chi\left(\frac{|v|}{\sqrt{T}}\right) v \, dv$$

$$(3.10) \quad \epsilon^B(\rho, p) = \int_0^{+\infty} \chi\left(\frac{|v|}{\sqrt{T}}\right) v^3 \, dv.$$

**Proof of Proposition 4.**

- Relations (3.3) and (2.10) show that

$$(3.11) \quad f^+(W) + \sigma f^-(W) = 0, \quad \sigma W = W.$$

Joined with relation (1.7), we have from relation (3.11)

$$(3.12) \quad f^+(W) - \sigma f^+(W) = f(W), \quad \sigma W = W$$

and relation (3.4) is established. Relation (3.5) is a direct consequence of (3.11).

- The detail of the computation of numerical viscosity is a consequence of relations (3.2), (3.4) and (3.5). □

**Proposition 5. Residual numerical viscosity.**

If one of the functions  $\mu(\bullet, \bullet)$  and  $\epsilon(\bullet, \bullet)$  explicitly depends on density, i.e. if we have

$$(3.13) \quad \frac{\partial \mu}{\partial \rho}(\rho, p) \neq 0 \quad \text{or} \quad \frac{\partial \epsilon}{\partial \rho}(\rho, p) \neq 0,$$

then the numerical viscosity of a flux vector splitting scheme is not infinitesimal for a stationary contact discontinuity, whatever be the size of the mesh.

**Proof of Proposition 5.**

- It is an immediate consequence of Proposition 4 and in particular of relation (3.6). □

**Proposition 6. Case of an approximate Riemann solver.**

Let  $\Phi(\bullet, \bullet)$  be one of the three exact or approximate Riemann solvers proposed by Godunov [Go59] (exact solution of the Riemann problem), Osher [Os81] (approximate solver containing only rarefaction waves or contact discontinuity) and Roe [Roe81] (approximate solver containing respectively only contact discontinuities). Then numerical viscosity  $V(W_l, W_r)$  of such a numerical scheme is null if given states  $W_l$  and  $W_r$  satisfy the particular conditions (1.9)-(1.10) of a stationary contact discontinuity.

### Proof of Proposition 6.

• In the case of Godunov and Osher schemes, conditions (1.9)-(1.10) state that the solution of the Riemann problem is effectively only composed by a stationary contact discontinuity. Due to Rankine-Hugoniot relations for a stationary discontinuity, physical fluxes of the two states  $W_l$  and  $W_r$  are equal and we have

$$(3.14) \quad f^* = (0, p, 0)^t = f(W_l) = f(W_r).$$

Taking into account Definition 2, the result is established in this case.

• If we use the Roe flux (without entropy fix, which is not necessary for a contact discontinuity, see for example [DM96]), we compute in a first step [Roe81] intermediate velocity  $u^*$  of a mean state :

$$(3.15) \quad u^* = \frac{\sqrt{\rho_l} u_l + \sqrt{\rho_r} u_r}{\sqrt{\rho_l} + \sqrt{\rho_r}} = 0$$

due to relation (1.9) and we evaluate also total enthalpy of this mean state before the calculus of of Roe matrix  $A^*$  that satisfies, taking into account (3.14) :

$$(3.16) \quad A^*(W_r - W_l) \equiv f(W_r) - f(W_l) = 0.$$

The difference  $(W_r - W_l)$  is an eigenvector of matrix  $A^*$  relatively to eigenvalue  $u^* = 0$  due to relation (3.15). In consequence, when we decompose discontinuity  $W_r - W_l$  on the basis of eigenvectors for matrix  $A^*$ , we observe that this difference is non null only for the linearly degenerated wave, i.e. on the contact discontinuity itself. Conclusion is then exactly the one done previously for Godunov and Osher fluxes.  $\square$

### 4) Conclusion.

• In order to capture numerically a boundary layer with a finite volume scheme, numerical analysis of the problem of stationary contact discontinuity shows that classical flux vector splitting schemes satisfying left-right invariance generates a numerical viscosity of order one relatively to the jump of densities whereas it is not the case if we use an exact or approximate decomposition of the Riemann problem. This fact founded on very simple algebra shows that Van Leer at al conclusion must be extended to all flux vector splittings referenced in this note : flux vector splitting is incompatible with viscous computations.

• This remark conducted us during the time of development of software Ns3gr [DM91] to include the Osher flux whereas the initial choice was Sanders and Prendergast flux vector splitting. This choice has been performing, even for resolution of Euler equations of gas dynamics in the particular case of

capturing shear stationary waves (see [DM92]). In an analogous way, the parabolized version Flu3pns (Chaput et al [Ch91]) of Flu3c computer software has required introduction of the Osher flux decomposition in order to simulate flows requiring a precise evaluation of viscous effects.

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