ON THE POSITIVITY OF FVS SCHEMES

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Abstract

Over the last ten years, robustness of schemes has raised an increasing interest among the CFD community. One mathematical aspect of scheme robustness is the positivity preserving property. At high Mach numbers, solving the conservative Euler equations can lead to negative densities or internal energy. Some schemes such as the flux vector splitting (FVS) schemes are known to avoid this drawback. In this study, a general method is detailed to analyze the positivity of FVS schemes. As an application, three classical FVS schemes (Van Leer's, Hänel's variant and Steger and Warming's) are proved to be positively conservative under a CFL-like condition. Finally, it is proved that for any FVS scheme, there is an intrinsic incompatibility between the desirable property of positivity and the exact resolution of contact discontinuities.

1. Introduction

In highly accelerated flows, the total energy is mainly composed of kinetic energy. Yet, in conservative formulation, both total and kinetic energy are computed independently, and their difference may yield negative internal energy, aborting the computation. In order to give some mathematical interpretation of schemes robustness or weakness in such severe configurations, it is useful to introduce the positivity property: a scheme is said to be positively conservative if, starting from a set of physically admissible states, it can only compute new states with positive densities and internal energies. Perthame (Perthame, 1990) first proposed a scheme which satisfies this property. Afterwards, Einfeldt *et al.*(Einfeldt, 1991) gave some results concerning Godunov-type schemes. They proved that Godunov scheme is positively conservative while Roe's scheme is not, and derived the HLLE method, a positive variant of HLL schemes family. Later, Villedieu and Mazet (Villedieu, 1995) proved that Pullin's EFM kinetic scheme (Pullin, 1980) is positively conservative under a CFL-like condition. Recently, Dubroca (Dubroca, 1998) proposed a positive variant of Roe's method. Since any scheme is positively conservative for a zero time step, it is absolutely essential to specify a time step condition when defining the positivity property.

2. Defining scheme positivity

Since one can formally extend any first-order one-dimensional positively conservative method to a second-order multidimensional positively conservative method (Perthame, 1996; Linde, 1997), we will restrict ourselves to the case of first-order schemes for the one-dimensional Euler equations in the following analysis. A conservative explicit method applied to the Euler equations can be expressed as

$$\mathbb{U}_i = \mathcal{U}_i - \frac{\Delta t}{\Delta x}\left[F_{i+1/2} - F_{i-1/2}\right] \tag{1}$$

where $\mathcal{U}_i$ is the average value over cell Ω_i of the vector of conservative variables ${}^T(\rho, \rho u, \rho E)$ at a given time step. $\mathbb{U}_i$ is the updated state vector. Δx is the measure of cell Ω_i and $F_{i+1/2}$ is the numerical flux between the cells Ω_i and Ω_{i+1}. The numerical flux is a function $F_{i+1/2} = F(\mathcal{U}_i, \mathcal{U}_{i+1})$ of the states in both neighboring cells. The numerical flux must satisfy the consistency condition $F(\mathcal{U}, \mathcal{U}) = \mathcal{F}(\mathcal{U})$, where $\mathcal{F}$ is the exact Euler flux. The discretized conservation equation Eq. (1) can be rewritten as

$$\mathbb{U}_i = \mathcal{U}_i - \frac{{\chi^{loc}}_i}{\lambda_i}\left[F_{i+1/2} - F_{i-1/2}\right] \tag{2}$$

where $\lambda(\mathcal{U})$ is the characteristic wave speed defined by $\lambda(\mathcal{U}) = |u| + a$ and ${\chi^{loc}}_i = \lambda(\mathcal{U}_i)\Delta t/\Delta x$. For physical reasons, the state $\mathcal{U}$ cannot take any arbitrary value in $\mathbb{R}^3$. Its density and internal energy must be both strictly positive. One can define $\Omega_{\mathcal{U}}$ as the open set of physically admissible states

$$\Omega_{\mathcal{U}} = \left\{\mathcal{U} = {}^T(u_1, u_2, u_3) \mid u_1 > 0 \text{ and } 2u_1u_3 - u_2^2 > 0\right\} \tag{3}$$

Vacuum is an admissible state for the closure $\overline{\Omega_{\mathcal{U}}}$ but not for $\Omega_{\mathcal{U}}$ since it is not expected to be reached in practical computations.

Definition 1 *A scheme is said to be* positively conservative *if and only if there exists a constant χ, such that if both conditions are satisfied*

$$\bullet \quad \forall i \in \mathbb{Z}\,, \quad \mathcal{U}_i \in \Omega_{\mathcal{U}} \tag{4a}$$

$$\bullet \quad \Delta t \leq \chi \frac{\Delta x}{\max\limits_{i \in \mathbb{Z}} \lambda(\mathcal{U}_i)} \tag{4b}$$

then

$$\forall i \in \mathbb{Z}\,, \quad \mathbb{U}_i \in \Omega_{\mathcal{U}} \tag{5}$$

For $\Delta t = 0$, according to Eq. (1), one has $\forall i \in \mathbb{Z}\,, \quad \mathbb{U}_i = \mathcal{U}_i \in \Omega_{\mathcal{U}}$ for any flux function used. So, for any continuous flux function F, since $\Omega_{\mathcal{U}}$ is an open subset of $\mathbb{R}^3$, whatever initial conditions $\mathcal{U}_i$ are in $\Omega_{\mathcal{U}}$, one can find Δt small enough which will preserve positivity of states $\mathbb{U}_i$. Consequently, the property of positivity consists of proving that Δt is not too small compared to the maximum time step given by the CFL condition. Otherwise, one can find a situation in which a physical admissible state can only be obtained by a vanishing time step, which is not acceptable for practical gas dynamics applications. On the contrary, a scheme is said to be *non-positive* if

$$\forall\, \chi > 0\,, \quad \exists\, (\mathcal{U})_{i \in \mathbb{Z}} \in \Omega_{\mathcal{U}}\,, \quad \mathbb{U}_i \notin \Omega_{\mathcal{U}} \tag{6}$$

For a non-positive scheme (e.g. Roe, AUSM), one may have to use an extremely small time step to update the solution and may not be able to produce a physically admissible solution after a finite period of time.

3. Positivity of FVS methods

This study has been restricted to a class of FVS schemes in which the fluxes $F^{\pm}$ satisfy the symmetry property

$$\overline{F^{-}(\mathcal{U})} = -F^{+}(\overline{\mathcal{U}}) \tag{7}$$

where $\overline{X}$ is the symmetric vector ${}^{T}(x_1, -x_2, x_3)$ of $X = {}^{T}(x_1, x_2, x_3)$. It should also satisfy

$$\forall u, a \in \mathbb{R} \times \mathbb{R}^{+}\,, \quad \lim_{\rho \to 0} F^{\pm}(\rho, u, a) = 0 \tag{8}$$

Since $F^{\pm}(\mathcal{U})$ is generally an homogeneous function of ρ, Eq. (8) is not a restrictive assumption in practice.

Theorem 1 *A given consistent FVS scheme satisfying properties (7) and (8) is positively conservative if and only if its $F^{\pm}$ functions satisfy both properties:*

- $\forall \mathcal{U} \in \Omega_{\mathcal{U}}\,, \quad F^{+}(\mathcal{U}) \in \overline{\Omega}_{\mathcal{U}}$ (9a)
- $\exists \chi > 0\,, \quad \forall \mathcal{U} \in \Omega_{\mathcal{U}}\,, \quad \mathcal{U} - \dfrac{\chi}{\lambda(\mathcal{U})}[F^{+}(\mathcal{U}) - F^{-}(\mathcal{U})] \in \overline{\Omega}_{\mathcal{U}}$ (9b)

In that case, the less restrictive positivity condition is expressed as

$$\forall i \in \mathbb{Z}\,, \quad {\chi^{loc}}_i < \chi_{opt} \tag{10}$$

where χ_{opt} is the greatest constant χ satisfying (9b).

Proof A detailed proof can be found in (Gressier, 1999).
The condition (9b) leads to a maximum time step which has then to be put into a CFL-like form $\chi^{loc} < \chi_{opt}$. This is the case for VL, VLH and SW schemes since $\chi_{opt} = \inf_M (\chi_{\max})$ is not zero. It turns out that the inter-

		VL	**VLH**	**SW**
F^{+}	Supersonic	$\lvert M\rvert \geq \sqrt{\dfrac{\gamma-1}{2\gamma}}$		
	Subsonic	$\gamma \geq 1$		$1 \leq \gamma \leq 3$
$\mathcal{W}_{\prime}$	Supersonic	$\chi^{loc} < \dfrac{\lvert M\rvert + 1}{\lvert M\rvert + \sqrt{\frac{\gamma-1}{2\gamma}}}$		
	Subsonic	$\chi^{loc} < \chi_{\max}^{VL}$	$\chi^{loc} < \chi_{\max}^{VLH}$	$\chi^{loc} < \chi_{\max}^{SW}$

TABLE 1. Internal energy positivity conditions

nal energy positivity conditions are always more stringent than the mass positivity conditions. Therefore, it is the internal energy positivity condition which actually drives the scheme positivity. Moreover, it means that zero values cannot be reached simultaneously by density and internal energy. Since expressions of $\chi_{\max}^{VL}$, $\chi_{\max}^{VLH}$ and $\chi_{\max}^{SW}$ are intricate, they are not detailed but these coefficients can be easily computed as a function of the local Mach number. The smallest values of these conditions have been computed and lead to the optimal CFL condition χ_{opt} which ensures that the scheme is positively conservative in all configurations. These constants χ_{opt} are summarized in table 2 and lead to an optimal CFL number of one for

VL	VLH	SW
1	$\min\left(1, \dfrac{2}{\gamma}\right)$	1

TABLE 2. Optimal CFL number χ_{opt}.

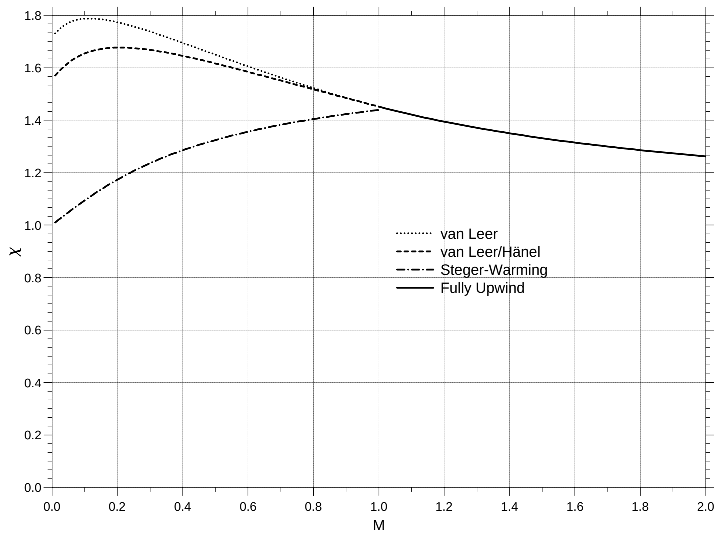

Figure 1. Maximum CFL number χ^{loc} to ensure internal energy positivity.

usual gases where $1 < \gamma < 2$. Since necessary and sufficient conditions have been derived, it can be interesting to plot the local CFL conditions. The different $\chi_{\max}$ functions are plotted on Fig. 1 for $\gamma = 1.4$. The SW scheme yields the most severe condition while the VL scheme allows a greater local CFL condition in the subsonic range. All three curves merge in the supersonic range where the CFL condition implies that χ should decrease to 1 for high Mach numbers (Fig. 1). As a consequence, a CFL number of one *a fortiori* ensures positivity of the three schemes. According to Fig. 1, a CFL number of 1.45 (for $\gamma = 1.4$) can be used with Van Leer's method if the flow is expected to remain subsonic. Note that this condition only ensures the scheme positivity, but not its stability. Using too high CFL numbers might produce oscillations even though the updated solution would still be an admissible state.

4. Accuracy versus Positivity

Most FVS schemes have proved to be robust in many flow configurations but none of them are able to exactly resolve contact discontinuities since it remains a non-vanishing dissipation which smears out an initial discontinuity of density. Van Leer (Van Leer, 1991) pointed out that preventing numerical diffusion of contact discontinuities may lead to a marginally stable or unstable behavior for slow flows.

Theorem 2 *If a FVS scheme exactly preserves stationary contact discontinuities, then it cannot be positively conservative.*

Proof Consider a FVS scheme given by its flux functions $F^{\pm}$, and assume it exactly preserves stationary contact discontinuities. Then, the interface flux between $\mathcal{U}_L = {}^T\left(\rho_L, 0, \frac{p}{\gamma-1}\right)$ and $\mathcal{U}_R = {}^T\left(\rho_R, 0, \frac{p}{\gamma-1}\right)$ must satisfy

$$F^+(\mathcal{U}_L) + F^-(\mathcal{U}_R) = (0,\ p,\ 0)^T \tag{11}$$

Since ρ_L and ρ_R are independent variables, $F^+(\mathcal{U}_L)$ must be a function of only p. Hence, for all $\mathcal{U} = {}^T\left(\rho, 0, \frac{p}{\gamma-1}\right)$,

$$F^+(\mathcal{U}) = (f_1(p),\ f_2(p),\ f_3(p))^T \tag{12a}$$

Moreover, considering the symmetry property (7) and using $\overline{\mathcal{U}} = \mathcal{U}$, one has $F^-(\mathcal{U}) = -\overline{F^+(\mathcal{U})}$. Then,

$$F^-(\mathcal{U}) = (-f_1(p),\ +f_2(p),\ -f_3(p))^T \tag{12b}$$

Substituting expressions (12a) and (12b) in Eq. (11), one obtains $f_2(p) = p/2$. Moreover, $f_1(p)$ must be positive or null to satisfy the condition (9a) of positivity. If $f_1(p) = 0$, condition (9a) is not satisfied since $f_2(p)$ is not null. If $f_1(p) > 0$, then the first component of $\mathcal{W}_I = \mathcal{U} - \dfrac{\chi^{loc}}{\lambda}[F^+(\mathcal{U}) - F^-(\mathcal{U})]$ may be expressed as

$$\rho - \frac{\chi^{loc}}{a} 2 f_1(p) = \rho - \sqrt{\rho}\left(2\chi^{loc}\frac{f_1(p)}{\sqrt{\gamma p}}\right) \tag{13}$$

Hence, for all functions $f_1(p)$ and for all $\chi^{loc} > 0$, one can always find p and ρ such that expression (13) is negative.

5. Conclusion

A general method to prove the positivity of FVS schemes has been proposed and applied to standard FVS schemes, namely the van Leer scheme, one of its variants, and the Steger and Warming scheme. Although these schemes have been known for a long time to be robust, they are now proved to be positively conservative under a CFL condition of 1, for usual values of the specific heat ratio γ in the range $[1;2]$. In particular, this shows that all these FVS schemes can be confidently applied to gas dynamics problems including real gas effects for which γ may range between 1.4 and 1. Moreover, these conditions have been proved to be incompatible with the particular form of FVS schemes which would be able to exactly preserve stationary contact discontinuities. In other words, one cannot develop a robust and accurate scheme within the FVS family.

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