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Numerical Analysis

Transport-equilibrium schemes for computing nonclassical shocks

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Abstract

This Note presents a very efficient numerical strategy for computing weak solutions of a scalar conservation law which fails to be genuinely nonlinear. In such a situation, the dynamics of shock solutions turns out to be mainly driven by a prescribed *kinetic function* that imposes the speed of propagation of the discontinuities. We show how to enforce the validity of the kinetic criterion at the discrete level. The resulting scheme provides, in addition, sharp profiles. Numerical evidence are included. ***To cite this article: C. Chalons, C. R. Acad. Sci. Paris, Ser. I 342 (2006).***

Résumé

Schémas transport-équilibre pour l'approximation des chocs nonclassiques. Cette Note présente un algorithme très efficace pour le calcul des solutions faibles d'une loi de conservation scalaire non vraiment nonlinéaire. Dans ce contexte, la dynamique des solutions choc repose principalement sur la donnée d'une *fonction cinétique* qui fixe la vitesse de propagation des discontinuités. Nous montrons comment forcer la validité du critère cinétique au niveau discret. Le schéma obtenu fournit par ailleurs des discontinuités sans diffusion numérique. Des résultats numériques sont présentés. ***Pour citer cet article : C. Chalons, C. R. Acad. Sci. Paris, Ser. I 342 (2006).***

1. Introduction

We are interested in computing nonclassical weak solutions of an initial-value problem for a scalar conservation law of the form

$$\begin{cases} \partial_t u + \partial_x f(u) = 0, \quad u(x,t) \in \mathbb{R}, \ (x,t) \in \mathbb{R} \times \mathbb{R}^{+*}, \\ u(x,0) = u_0(x), \end{cases} \tag{1}$$

where $f:\mathbb{R} \to \mathbb{R}$ is a (smooth) *nonconvex* flux-function. Generally speaking, solutions of problem (1) may be discontinuous and are not uniquely determined by initial data u_0. According to a general regularization principle, we thus ask solutions of (1) to satisfy a single entropy inequality of the form

$$\partial_t U(u) + \partial_x F(u) \leqslant 0, \tag{2}$$

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where $U:\mathbb{R}\to\mathbb{R}$ and $F:\mathbb{R}\to\mathbb{R}$ are *specified* functions such that U is strictly convex and $F'=U'f'$. When f is convex, entropy condition (2) actually selects a unique *classical* solution of (1). When f fails to be convex, it is necessary to supplement (1)–(2) with an additional selection criterion called *kinetic relation* from [4]. More precisely, the Riemann problem associated with (1)–(2) still admits a one-parameter family of solutions, which may contain shock waves violating Lax shock inequalities. Such discontinuities are referred as to *undercompressive shocks* or *nonclassical shocks*. In order for the uniqueness to be ensured, a *kinetic relation* needs to be added along each nonclassical discontinuity connecting a left state u_- to a right state u_+. It takes the form $u_+=\varphi^\flat(u_-)$ or $u_-=\varphi^{-\flat}(u_+)$ where $\varphi^\flat$ is the so-called *kinetic function* and $\varphi^{-\flat}$ its inverse. We refer to [4] for a general theory of nonclassical entropy solutions.

The numerical approximation of nonclassical solutions is known to be very challenging. The main difficulty is the respect of the kinetic relation at the discrete level. At once, such nonclassical solutions are actually present in real and complex problems coming from the physics. Let us mention for instance the study of compressible fluids undergoing vapor-liquid phase changes, which is our main motivation.

In this Note, we present a new scheme for capturing discontinuities whose dynamics is driven by a kinetic function. Our strategy deals directly with the kinetic function $\varphi^\flat$ to tackle the nonclassical solutions. The resulting algorithm provides numerical results in full agreement with exact ones, whatever the strength of the shocks are. In particular, our scheme leaves sharp isolated nonclassical shocks.

2. The case of cubic flux and nonclassical Riemann solver

Without loss of generality, we take $f(u)=u^3$ which is to some extent the simplest example of a nonconvex function, and refer to [1] for more general flux functions. We consider weak solutions of (1) satisfying entropy inequality (2) with $U(u)=u^2$ and $F(u)=\frac{3}{4}u^4$, and choose (again without restriction) $\varphi^\flat(u)=-\beta u$ as a kinetic function, with $\beta\in[1/2,1)$ so that each nonclassical shock obeys (2).

Given two constant states u_l, u_r such that $u_l>0$, we consider a Riemann initial data u_0 defined by $u_0(x)=u_l$ if $x<0$ and $u_0(x)=u_r$ if $x>0$. Following [4] and defining $\varphi^\sharp(u)=-u-\varphi^\flat(u)$, the solution of (1)–(2), supplemented with the kinetic criterion associated with $\varphi^\flat$, is given as follows:

(1) If $u_r\geqslant u_l$, the solution is a rarefaction wave connecting u_l to u_r.
(2) If $u_r\in[\varphi^\sharp(u_l),u_l)$, the solution is a classical shock wave connecting u_l to u_r.
(3) If $u_r\in(\varphi^\flat(u_l),\varphi^\sharp(u_l))$, the solution contains a nonclassical shock connecting u_l to $\varphi^\flat(u_l)$, followed by a classical shock connecting $\varphi^\flat(u_l)$ to u_r.
(4) If $u_r\leqslant\varphi^\flat(u_l)$, the solution contains a nonclassical shock connecting u_l to $\varphi^\flat(u_l)$, followed by a rarefaction connecting $\varphi^\flat(u_l)$ to u_r.

3. Numerical approximation

We now present a suitable algorithm for approximating these Riemann solutions. Let be given a time step Δt and a space step Δx. Introducing $x_{j+1/2}=j\Delta x$ for $j\in\mathbb{Z}$ and $t^n=n\Delta t$ for $n\in\mathbb{N}$, we seek at each time t^n an approximation u_j^n of u on each interval $[x_{j-1/2};x_{j+1/2})$. In this context, we choose without restriction a two-point numerical flux function $g:(u,v)\to g(u,v)$ consistent with the flux function f.

Let us first motivate our algorithm. Actually, it is observed in [1,2] that a classical conservative scheme associated with g is not able to propagate any isolated nonclassical shock. Instead, some *spurious* values are created by the scheme, eventually leading to a damaged numerical solution. Our algorithm aims at removing these *spurious* values. This is achieved in the first step of the method by systematically making stationary the nonclassical discontinuities. Which means in particular that the conservation property is lost, so that the use of a nonconservative update formula is completely natural in this first step. Then, the dynamics of the nonclassical discontinuities is taken into account in the second step of the strategy, thus restoring (in a weak sense) the conservation property.

First step ($t^n\to t^{n+1-}$) As motivated above, this step aims at making stationary the nonclassical discontinuities of our problem. For that, we introduce the following nonconservative update formula:

$$u_j^{n+1-}=u_j^n-\lambda\big(g_{j+1/2}^L-g_{j-1/2}^R\big),\quad j\in\mathbb{Z},\ \text{with } \lambda=\Delta t/\Delta x, \tag{3}$$

where the numerical fluxes $g^L_{j+1/2}$ and $g^R_{j+1/2}$ have to be suitably defined. In this note, we will focus ourselves on the numerical approximation of the nonclassical discontinuities only (the most difficult ones to capture numerically), that is those separating two states u_- and u_+ such that $u_+ = \varphi^\flat(u_-) < \varphi^\sharp(u_-)$ when $u_- > 0$. Then, it is easily checked that defining $g^L_{j+1/2}$ and $g^R_{j+1/2}$ as follows when $u^n_j > 0$:

$$g^L_{j+1/2} = \begin{cases} g(u^n_j, \varphi^{-\flat}(u^n_{j+1})) & \text{if } u^n_{j+1} < \varphi^\sharp(u^n_j), \\ g(u^n_j, u^n_{j+1}) & \text{otherwise,} \end{cases} \tag{4}$$

$$g^R_{j+1/2} = \begin{cases} g(\varphi^\flat(u^n_j), u^n_{j+1}) & \text{if } u^n_{j+1} < \varphi^\sharp(u^n_j), \\ g(u^n_j, u^n_{j+1}) & \text{otherwise,} \end{cases} \tag{5}$$

and, in a first approach at least, equal to $g_{j+1/2}$ when $u^n_j \leqslant 0$ (see [1] for details) is sufficient to keep at stationary equilibrium all the discontinuities separating two states u_- and u_+ such that $u_+ = \varphi^\flat(u_-)$.

Second step ($t^{n+1-} \to t^{n+1}$) This step deals with the dynamics of the nonclassical discontinuities left stationary during the first step. We first recall that the speed of propagation $\sigma(u_-, u_+)$ of a discontinuity between u_- and u_+ is given by Rankine–Hugoniot conditions, that is $\sigma(u_-, u_+) = [f(u_+) - f(u_-)]/[u_+ - u_-]$. We then define at each interface $x_{j+1/2}$ a speed of propagation $\sigma_{j+1/2}$ by

$$\sigma_{j+1/2} = \begin{cases} \sigma(u^{n+1-}_j, u^{n+1-}_{j+1}) & \text{if } u^n_{j+1} < \varphi^\sharp(u^n_j), \\ 0 & \text{otherwise,} \end{cases} \tag{6}$$

and solve at each discontinuity $x_{j+1/2}$ a transport equation with speed $\sigma_{j+1/2}$. In order to avoid the appearance of new *spurious* values and to get a new approximation u^{n+1}_j at time $t^{n+1} = t^n + \Delta t$, we propose to pick up randomly on interval $[x_{j-1/2}, x_{j+1/2}[$ a value in the juxtaposition of these Riemann solutions at time Δt chosen small enough to avoid wave interactions. Given a well distributed random sequence (a_n) within interval $(0, 1)$, it amounts to set:

$$u^{n+1}_j = \begin{cases} u^{n+1-}_{j-1} & \text{if } a_{n+1} \in [0, \lambda\sigma^+_{j-1/2}[, \\ u^{n+1-}_j & \text{if } a_{n+1} \in [\lambda\sigma^+_{j-1/2}, 1 + \lambda\sigma^-_{j+1/2}[, \\ u^{n+1-}_{j+1} & \text{if } a_{n+1} \in [1 + \lambda\sigma^-_{j+1/2}, 1[, \end{cases} \quad \text{with} \begin{cases} \sigma^-_{j+1/2} = \min(\sigma_{j+1/2}, 0), \\ \sigma^+_{j-1/2} = \max(\sigma_{j-1/2}, 0). \end{cases} \tag{7}$$

4. Numerical experiments

We give two numerical evidences to validate our scheme. We take a Roe scheme as a basic numerical flux g, and the van der Corput random sequence for (a_n). For the kinetic function $\varphi^\flat$, we set $\beta = \frac{3}{4}$. We consider the typical nonclassical behaviors of the Riemann solution given in Section 2, when taking $u_l = 4$ and u_r equal to -2 (test 1) or -5 (test 2). Numerical solutions are plotted on Fig. 1 for $\Delta x = 10^{-2}$.

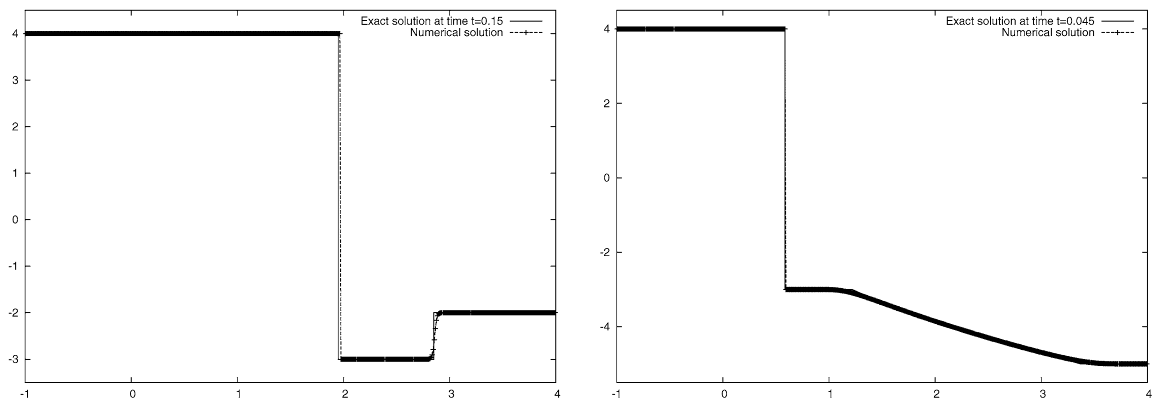

Fig. 1. Nonclassical solutions: test 1 (left) and test 2 (right).

Fig. 1. Solutions nonclassiques : test 1 (gauche) et test 2 (droite).

We observe that the numerical solutions fully agree with the exact ones. In particular, the right states of the nonclassical waves are exactly captured, which is remarkable, while there are not any points in their profile (see [1] and the references therein). For test 1, we note that the classical shock contains some numerical diffusion induced by the Roe scheme. In [1], we show how to slightly modify the definitions of the numerical fluxes $g^L_{j+1/2}$ and $g^R_{j+1/2}$ in (4)–(5) in order to make sharp the classical shocks, too.

To conclude, an efficient numerical strategy has been presented for computing nonclassical solutions of a particular scalar conservation law. It provides sharp nonclassical interfaces propagating at the right speed whatever the strength of interfaces are. The method turns out to be nonconservative but measures in [1] have shown that the loss of conservation is extremely low, while numerical solutions fully agree with exact ones. We emphasize that our approach is built *without explicitly using the knowledge of the underlying nonclassical Riemann solver*, contrary to Glimm's method for instance. Which means that it is not an expensive method and that it may be used for more complex applications. An application to pedestrian flows has been addressed in [2]. In [3], we consider the case of a hyperbolic-elliptic model with phase changes that has initially motivated the present study.

References

[1] C. Chalons, Transport-Equilibrium schemes for computing nonclassical shocks. I. Scalar conservation laws, Laboratoire J.-L. Lions, Preprint R05031, 2005. Available at http://www.ann.jussieu.fr.

[2] C. Chalons, Numerical approximation of a macroscopic model of pedestrian flows, Laboratoire J.-L. Lions, Preprint R05032, 2005. Available at http://www.ann.jussieu.fr.

[3] C. Chalons, Transport-equilibrium schemes for computing nonclassical shocks, II. A hyperbolic-elliptic model of phase transitions, in preparation.

[4] P.G. LeFloch, Hyperbolic Systems of Conservation Laws: The Theory of Classical and Nonclassical Shock Waves, E.T.H. Lecture Notes Series, Birkhäuser, 2002.