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NUMERICAL MODELLING OF POLLUTANT TRANSPORT

A. Balaguer, E. D. Fernández-Nieto, B. Latorre and V. Martínez

Abstract. In this work we study an artificial compression technique to treat discontinuities associated to linearly degenerated fields, with application to pollutant transport. The basic idea is to introduce a new flux in order to solve a new equation where the contact discontinuity is now a shock, travelling to the same velocity. We propose a flux-limiter method that combines the artificial compression technique and two second order methods. This method allows to apply the artificial compression technique in all the domain, without detecting the discontinuity jumps. We present a 2D test where the improvement of the presented technique can be observed.

Keywords: Artificial compression, pollutant transport, flux-limiters methods.

AMS classification: 65M05, 65M10.

§1. Introduction

A scalar conservation law, under certain regularity hypotheses, reduces to the partial differential equation

$$\begin{cases} u(x,t)_t + f(u(x,t))_x = 0, & (x,t) \in \mathbb{R} \times \mathbb{R}^+, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1}$$

where $u : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ is the conserved variable and $f : \mathbb{R} \to \mathbb{R}$ is the flux function.

The pollutant transport is associated to linearly degenerated fields. If a is the velocity of the fluid, the pollutant concentration is the solution of the an advection equation

$$u_t + a u_x = 0. \tag{2}$$

In the case that a is contant, the profile of the pollutant concentration can present contact discontinuities. The problem of the pressence of contact discontinuities is that they have a numerical diffusion more marked that shocks present in equations with non linear flux.

Harten presents a technique to treat this type of discontinuities in the pioneering work [3], dated in 1977 and in which some modifications of standard finite differences methods are discussed. Latter in 1989, Harten [4] again introduced the novel concept of subcell resolution.

Recently, the artificial compression method has been employed to improve the numerical solution of a great number of problems by using a great variety of techniques. For example, Yang [2], Lie and Noelle [5]. A brief description of the state of the art of this subject can be found in [1].

When the initial data of the problem has two constant states

$$u_0(x) = \begin{cases} u_-, & x < x_d, \\ u_+, & x > x_d. \end{cases} . \tag{3}$$

Martínez and Fernández-Nieto (see [6] and [1]) propose a procedure of artificial compression based on a modification of the flux to obtain a better numerical approach in the jumps of the solution. The idea is to detect the jump and to replace in this zone the linear flux in equation (2) by a nonlinear flux, so that the analytical solution in the original equation is conserved [6].

The objective of this work is to apply this technique to a second order scheme and to avoid the step of detection of discontinuity jumps. In Section 2 we propose a flux-limiter method based in the use of the compression technique and the combination of two second order methods. This method allows us to avoid the step of detection of discontinuity jumps and to improve the results of the second order methods. Finally, in Section 3 we present two numerical tests.

§2. Flux-limiter upwind method with artificial compression

In this section we first present a flux-limiter method that combines the first order upwind method with a second order one. For the second order method we present two possibilities: the classical Lax-Wendroff scheme (LW in what follows) and the second order upwind scheme (UP2 in what follows). After, we propose another scheme that uses a random combination of these two second order methods.

Numerical schemes using flux limiters can be defined by

$$\bar{u}_j^{n+1} = \bar{u}_j^n - \frac{\Delta t}{\Delta x}(\phi_{j+1/2}^n - \phi_{j-1/2}^n), \tag{4}$$

where

$$\phi_{j+1/2}^n = \phi_{j+1/2}^{1st} + \varphi(r_{j+1/2}^{2nd})(\phi_{j+1/2}^{2nd} - \phi_{j+1/2}^{1st}). \tag{5}$$

By $\phi_{j+1/2}^{1st}$ and $\phi_{j+1/2}^{2nd}$ we denote the numerical flux functions of first and second order respectively at time $t = t^n$. By $\varphi(r^{2nd})$ we denote a flux limiter function, which is defined in function of a non-dimensional quantity: r^{2nd}. The definition of r^{2nd} depends on the choice of the second order method. For the first order method we consider the upwind scheme:

$$\phi_{j+1/2}^{1st} = \frac{f(u_j) + f(u_{j+1})}{2} - \frac{1}{2}\,|a_{j+1/2}|\,(u_{j+1} - u_j), \tag{6}$$

where $a = \partial_u f$. And the compressed first order method reads

$$\phi_{j+1/2}^{1st,comp} = \frac{\tilde{f}(u_j) + \tilde{f}(u_{j+1})}{2} - \frac{1}{2}\left|\partial_u \tilde{f}_{j+1/2}\right|(u_{j+1} - u_j), \tag{7}$$

where $\tilde{f}(u)$ is defined by using an artificial compresion technique as follows. Following [1] we consider the flux

$$\tilde{f}(u) = au + g(u), \tag{8}$$

where

$$g(u) = \rho(u - u_-)(u - u_+), \tag{9}$$

where ρ is a parameter, which is chosen to assure the dynamical consistency of the jump (see [6] and [1]). It must verify:

$$\rho > 0, \text{ if } u_- > u_+ \quad \text{and} \quad \rho < 0, \text{ if } u_- < u_+. \tag{10}$$

In [6] it is proved that, if we consider a numerical scheme stable under a CFL condition λ_0 and if

$$|\rho| \leq \frac{\lambda_0 - |a| \frac{\Delta t}{\Delta x}}{\frac{\Delta t}{\Delta x} |u_- - u_+|}, \tag{11}$$

then the numerical scheme is also stable for the modified flux under the same CFL condition. For the numerical schemes that we consider in this work we have $\lambda_0 = 1$.

By $\partial_u \tilde{f}_{j+1/2}$ we denote the Roe average, that verifies

$$\tilde{f}(u_{j+1}) - \tilde{f}(u_j) = (\partial_u \tilde{f}_{j+1/2})(u_{j+1} - u_j). \tag{12}$$

As we mentioned previously, we consider two different possibilities for the second order method:

- Lax-Wendroff (LW):

$$\phi^{LW}_{j+1/2} = \frac{f(u_j) + f(u_{j+1})}{2} - \frac{1}{2}\frac{\Delta t}{\Delta x} a_{j+1/2}(f(u_{j+1}) - f(u_j)). \tag{13}$$

For Lax-Wendroff method $r^{2nd} = r^{LW}$ is defined by

$$r^{LW} = \begin{cases} (u_j - u_{j-1})/(u_{j+1} - u_j), & \text{if } a_{j+1/2} > 0, \\ (u_{j+1} - u_j)/(u_j - u_{j+1}), & \text{if } a_{j+1/2} < 0. \end{cases} \tag{14}$$

- Upwind second order ($UP2$):

$$\begin{aligned} \phi^{UP2}_{j+1/2} = \frac{1}{2}\Bigg(& f(u_j) + f(u_{j+1}) - \left|a_{j+1/2}\right| (u_{j+1} - u_j) \\ & + (1 - \lambda a^+_{j-1/2}) \frac{1 + \operatorname{sgn}(a_{j-1/2})}{2} (f(u_j) - f(u_{j-1})) \\ & - (1 + \lambda a^-_{j+3/2}) \frac{1 - \operatorname{sgn}(a_{j+3/2})}{2} (f(u_{j+2}) - f(u_{j+1})) \Bigg), \end{aligned}$$

where $a^\pm = (a \pm |a|)/2$. In this case $r^{2nd} = r^{UP2}$ is defined by

$$r^{UP2} = \begin{cases} (u_j - u_{j+1})/(u_{j-1} - u_j), & \text{if } a_{j+1/2} > 0, \\ (u_{j+1} - u_j)/(u_{j+2} - u_{j+1}) & \text{if } a_{j+1/2} < 0. \end{cases} \tag{15}$$

Finally, we present another numerical scheme based in a combination of previous one and the compression technique. The objective is to propose a new numerical scheme that improves previous second order methods, by using the artificial compression proposed technique, and to omit the detection of the discontinuity jump, that is, to apply the compression in all the domain without a conditionally jump detection.

The numerical flux function is

$$\phi_{j+1/2} = \phi_{j+1/2}^{1st,comp} + \varphi(r_{j+1/2}^{2nd})(\phi_{j+1/2}^{2nd} - \phi_{j+1/2}^{1st,comp}). \tag{16}$$

By $\phi_{j+1/2}^{1st,comp}$ we denote the numerical flux function of the first order upwind method applying the artificial compression technique (7). By $\phi_{j+1/2}^{2nd}$ we denote a second order method, for example LW or UP2. And by $\varphi(r)$ a flux-limiter function. For the numerical tests we have considered the minmod flux-limiter function.

Observe that the purpose to use flux-limiters functions is to combine two methods by applying the first order one near discontinuities and the second order one outside discontinuities. So, by applying the compression technique for the first order method only, we can omit the detection of discontinuity jumps.

Another improvement is the choice of the second order method. Instead of consider LW or UP2, we propose a combination of them. One possibility is to define $\phi_{j+1/2}^{2nd}$ as the mean average of LW and UP2. But in this case we must compute both fluxes. Another possibility is to choice in each intercell $j + 1/2$, one of them, for example we can use a random function to select of them. We have compared both possibilities for tests 4 and 5 and the final results are nearly the same. Then we only show the results corresponding to the cheaper possibility, the random choice.

The motivation to use a combination of LW and UP2 methods is illustrated in tests 1 and 2. We can observe that the results obtained by using the flux-limiter version with the LW and the UP2 method present a symmetrical and opposite behavior near discontinuities (see for example Figures 1(b) and 1(c)).

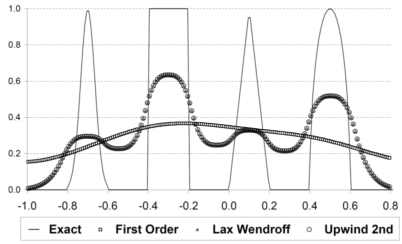
The artificial compression technique presented in the paper can be easily extended to 2D domains (see [1]). Basically, the finite volume method for 2D equations is based into apply a 1D flux at each edge of the 2D control volume. In test 2, we consider the same proposed combination using flux function (16), by combining the compressed first order upwind method, the 2D LW method and the 2D UP2 method.

§3. Numerical tests

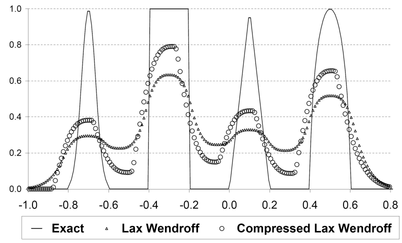
3.1. Test 1: four profiles

We consider the following problem:

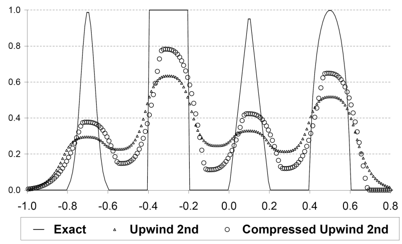
$$\begin{cases} u_t + u_x = 0, \quad -1 \le x \le 1, \\ u_0(x) = \begin{cases} e^{(\ln 2)\,(x+0.7)^2/0.0009}, & -0.8 \le x \le -0.6, \\ 1, & -0.4 \le x \le -0.2, \\ 1 - |10x - 1|, & 0 \le x \le 0.2, \\ \sqrt{1 - 100(x - 0.5)^2}, & 0.4 \le x \le 0.6, \\ 0, & \text{otherwise.} \end{cases} \end{cases} \tag{17}$$



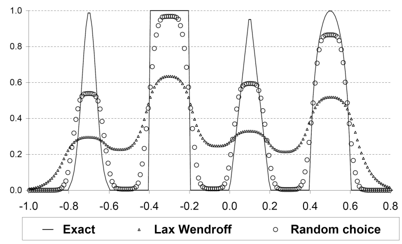
(a) First order, LW, upwind second order



(b) LW and compressed LW



(c) Upwind second order and compressed upwind second order



(d) LW and compressed random choice

Figure 1: Test 1, comparison of first order, compressed Lax-Wendoff, compressed upwind second order and compressed random choice method.

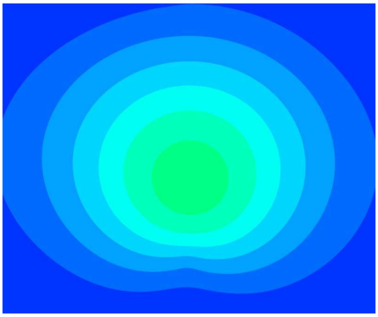
We consider $NX = 200$ points in $[-1, 1]$ and periodic boundary conditions. The final time is $t = 20$, and by the CFL condition we set $(\Delta t/\Delta x) = 0.5$. In Figure 1 we compare the results obtained with the first order upwind method (Figure 1(a)), the second order flux-limiter version with LW scheme (Figure 1(b)), the UP2 version (Figure 1(c)) and the proposed scheme (16), by using a random combination of LW and UP2 (Figure 1(d)). We observe that the less diffusive method is the proposed compressed random choice method. It improves the results for all the profiles.

3.2. Test 2: 2D test

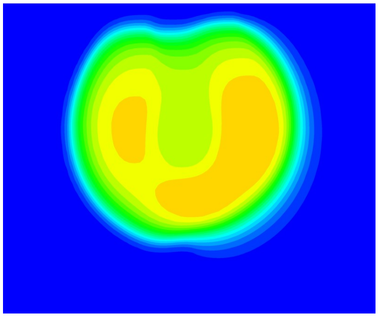
In this subsection we consider a 2D problem, where the domain is $[0, 1]\times[0, 1]$. We discretize the domain in quadrangular cells, with $NX = NY = 200$. We consider the following problem:

$$\begin{cases} u_t + a(x,y)\, u_x + b(x,y)\, u_y = 0, \quad 0 \le x \le 1, \quad 0 \le y \le 1, \\ u_0(x,y) = \begin{cases} 1, & \text{if } (x,y) \in \Omega^1, \\ 0, & \text{otherwise,} \end{cases} \end{cases} \tag{18}$$

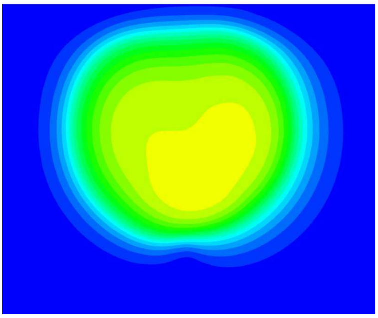
where Ω^1 is defined by the points (x, y) of the circle of ratio $r = 0.2$ and center $(0.5, 0.75)$, which are external to the rectangle $[0.475, 0.525] \times [0.65, 1]$.



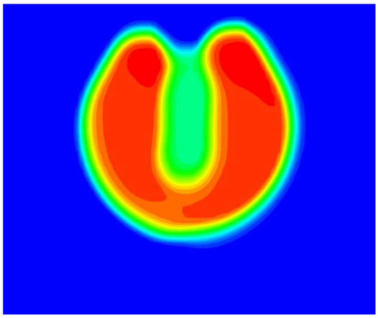
(a) Upwind



(b) Lax-Wendroff



(c) Upwind second order



(d) Random choice

Figure 2: Test 2, t=4. (a) Upwind, (b) Flux limiter method with Lax-Wendroff, (c) Flux limiter method with Upwding second order (d) Random choice.

The velocity field is defined by a circular champ centered in $(0.5, 0.5)$:

$$a(x,y) = -2\pi(y-0.5), \quad b(x,y) = 2\pi(x-0.5). \tag{19}$$

Then, the test consist in a profile that is transported circularly around the center of the domain, $(0.5, 0.5)$. The time necessary to give a compleat turn is a period $T = 1$. By the CFL condition we set $(\Delta t/\Delta x) = \sqrt{2}/(4\pi)$.

In Figure 2 we present the level curves corresponding to the calculated profile at $t = 4T$. Figure 2(a) corresponds to the numerical result with the first order upwind method. Figure 2(b) corresponds to the LW with flux limiter scheme. Figure 2(c) corresponds to the UP2 method. And Figure 2(d) corresponds to the proposed scheme (16) in 2D. We observe that the proposed scheme present less diffusion in the four times presented.

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A. Balaguer
Departamento de Matemática Aplicada,
Universidad Politécnica de Valencia,
E.T.S.I. Geodésica, Cartográfica y Topográfica,
Camino de Vera s/n, 46022 Valencia, Spain
abalague@mat.upv.es

E. D. Fernández-Nieto
Departamento de Matemática Aplicada I,
Universidad de Sevilla. E.T.S. Arquitectura.
Avda, Reina Mercedes, s/n. 41012 Sevilla, Spain
edofer@us.es

B. Latorre
Departamento de Mecánica de Fluidos,
Universidad de Zaragoza
Centro Politécnico Superior
María de Luna 3. 50015 Zaragoza, Spain
borja.latorre@unizar.es

V. Martínez
Departamento de Matemáticas
Universitat Jaume I,
Campus de Riu Sec, 12071 Castelló, Spain
martinez@mat.uji.es