

Construction of conservative PkPm space-time residual discretizations for conservation laws I: theoretical aspects

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Key-words: conservation laws, time dependent problem, high order, positivity preservation, nonlinear schemes, residual distribution

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1 Generalities

We want to approximate solutions of the nonlinear conservation law

$$\partial_t u + \partial_x f(u) = 0 \quad \text{on} \quad [0, L] \times [0, T] \subset \mathbb{R} \times \mathbb{R}^+ \quad (1)$$

System (1) is assumed to be embedded with a set of boundary and initial conditions, and to verify all the classical assumptions : existence of an entropy pair, symmetrizability, hyperbolicity, etc...

1.1 Discrete equations

There is nowadays a large number of techniques allowing to deal with (1) numerically. We can mention among them the Discontinuous Galerkin method [12] and its implicit space-time [6, 33, 26] and explicit variants [29, 16, 19], the spectral finite volume and finite difference schemes [35, 36, 37], high order WENO [30] and residual based finite volume schemes [13, 14, 9, 10], to cite some.

The main issues to be dealt with when solving (1) numerically are the following :

Discrete conservation Across a discontinuity moving at speed σ , the discrete equations should consistently approximate the Rankine-Hugoniot relation

$$\sigma[u] = [f] \quad (2)$$

having denoted by $[\cdot]$ the jumps across the discontinuity ;

Positivity, non-oscillatory character No unphysical numerical oscillations should be produced in correspondence of discontinuities. Also for components of u under a strict positivity constraint (as commonly density, pressure or temperature), the non-negativity of these components should be guaranteed when they go to zero (*e.g.* when a domain of void is generated) ;

Time step size The above positivity condition is often achieved under a constraint on the time step size [8, 20]. This can be a flaw, especially if the underlying discretization is implicit in time [28]. High order positivity preserving schemes for (1) should be either explicit, or unconditionally (w.r.t. the time step) positivity preserving ;

Accuracy It should be possible to increase arbitrarily the accuracy measured in practice in correspondence of a smooth solutions, both in space and in time ;

To the authors' knowledge, no existing method allows to retain *all* of the above properties in practical computations. In this paper we propose an approach allowing to obtain such a scheme.

2 The space-time residual approach

The schemes considered are inspired by the Residual Distribution (RD) schemes [15, 1, 28]. The formulation proposed here, however, is a genuinely Petrov-Galerkin method with test functions defined in such a way that the standard RD schemes are recovered in the P^1 case.

In particular, we generalize the work of [21, 22] on space-time RD schemes with discontinuous time representation. This generalization is obtained by means of

1. a high order $P^n P^m$ interpolation in space-time ;
2. a Petrov-Galerkin variational setting inspired by principles similar to those used in RD schemes ;
3. a space-time conservative formulation via a $P^{k+1} P^m$ reconstruction of the flux divergence ;
4. a positivity preserving approach based on the Limited Lax-Friedrich's scheme of [28] .

The above items are discussed in the following sections.

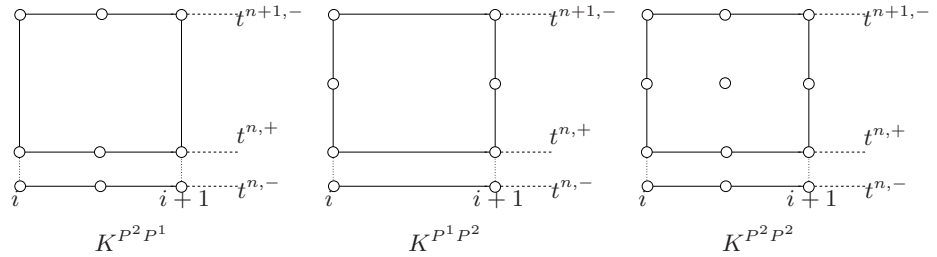


Figure 1: Examples of $P^n P^m$ elements

2.1 Space-time approximation

We discretize the one-dimensional spatial domain $[0, L]$ by means of a set of non-overlapping elements

$$\Omega_h = \bigcup_{i=1}^N [i, i+1] = \bigcup_{i=1}^N K_i,$$

having set $K_i = [i, i+1]$, and the temporal domain $[0, T]$ by means of a set of non-overlapping time slabs

$$\mathcal{T}_{\Delta t} = \bigcup_{n=1}^M [t^n, t^{n+1}] = \bigcup_{n=1}^M K^n.$$

having set $K^n = [t^n, t^{n+1}]$. We also set

$$h = \min_i (x_{i+1} - x_i), \quad \Delta t = \min_n (t^{n+1} - t^n)$$

In the space-time slab $[0, L] \times [t^n, t^{n+1}]$ we consider space-time elements $K_i^n = K_i \times K^n = [i, i+1] \times [t^n, t^{n+1}]$. Over each K_i^n we introduce a polynomial representation of the unknown, which we denote by u_h . In order to do this, within each K_i^n we consider $\{\varphi_j^s(x)\}_{j=1}^{k+1}$ and $\{\varphi_l^t(t)\}_{l=1}^{m+1}$, the standard one dimensional Lagrange basis functions on equally spaced points, of polynomial degree k and m respectively. While we assume a *continuous approximation in space*, so that the local values $u_j(t)$ are uniquely defined, *the approximation in time is discontinuous*, hence the value $u^n(x)$ is not uniquely defined. In particular, as shown on figure 1, at the generic time level t^n we define the limits

$$u_h^{n,-}(x) = \sum_{K_i} \sum_{j=1}^{k+1} \varphi_j^s(x) u_j^{n,-}, \quad u_h^{n,+}(x) = \sum_{K_i} \sum_{j=1}^{k+1} \varphi_j^s(x) u_j^{n,+} \quad (3)$$

and the jump

$$[u_h]^n(x) = \sum_{K_i} \sum_{j=1}^{n+1} \varphi_j^s(x) [u_j]^n, \quad [u_j]^n = u_j^{n,+} - u_j^{n,-} \quad (4)$$

With this notation, within each K we define the local approximation

$$u_h|_{K_i^n} = u_h^{n,+}(x) + \sum_{j=1}^{k+1} \sum_{2 \leq l \leq m} \varphi_j^s(x) \varphi_l^t(t) u_j^l + u_h^{n+1,-}(x) \quad (5)$$

As illustrated on figure 1 this leads to the adoption of $P^k P^m$ tensor product elements in space-time.

2.2 Petrov-Galerkin setting and space-time conservation

Given the values $\{u_j^{n,-}\}_{j \in \Omega_h}$, the values of the degrees of freedom in the slab $\Omega_h \times [t^{n,+}, t^{n+1,-}]$ are computed by means of the variational statement

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^l(x, t) (\partial_t u_h + \partial_x f_h(u_h)) = 0, \quad \forall j \in \Omega_h \text{ and } \forall 1 \leq l \leq m+1 \quad (6)$$

with $f_h(u_h)$ a discrete approximation of the flux, and where β_j^l is a Petrov-Galerkin test function, assumed to be uniformly bounded w.r.t. h , Δt , u_h , and w.r.t. the local residuals $\{(\partial_t u_h + \nabla \cdot f_h(u_h))|_{K_i^n}\}_{\forall i,n}$, and locally differentiable. The test functions are also assumed to verify the consistency condition

$$\sum_{j=1}^{k+1} \sum_{l=1}^{m+1} \beta_j^l = 1 \quad (7)$$

Statement (6) does not take into account the discontinuous nature of the temporal approximation. To do that, we integrate (6) by parts introducing the upwind numerical flux $\hat{u}_h^n(x) = u_h^{n,-}(x)$, in equations :

$$\begin{aligned} 0 &= - \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t} K_i^n} \int (\partial_t \beta_j^l(x, t) u_h) |_{K_i^n} + \int_{\Omega_h} (\beta_j^l(x, t^{n+1,-}) \hat{u}_h^{n+1} - \beta_j^l(x, t^{n,+}) \hat{u}_h^n) \\ &\quad + \int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^l(x, t) \partial_x f_h(u_h) = \\ &= - \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t} K} \int (\partial_t \beta_j^l(x, t) u_h) |_{K_i^n} + \int_{\Omega_h} (\beta_j^l(x, t^{n+1,-}) u_h^{n+1,-} - \beta_j^l(x, t^{n,+}) u_h^{n,-}) \\ &\quad + \int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^l(x, t) \partial_x f_h(u_h) \end{aligned}$$

We now add and subtract in the second integral the quantity $\beta_j^l(x, t^{n,+}) u_h^{n,+}$ and integrate by parts over each K again to obtain the final Petrov-Galerkin form of the scheme

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^l(x, t) (\partial_t u_h + \partial_x f_h(u_h)) + \int_{\Omega_h} \beta_j^l(x, t^{n,+}) [u_h(x)]^n = 0, \quad \forall j \in \Omega_h \text{ and } \forall 1 \leq l \leq m+1 \quad (8)$$

The name of the game is now to find definitions of the test functions β_j^l and of the traces $\beta_j^l(x, t^{n,+})$ yielding the desired properties.

Independently on this definition, it is important to remark that, provided that the discrete flux $f_h(u_h)$ is continuous in space, statement (8) is globally conservative. This can be easily shown by noting that when testing the scheme with functions $\beta_j^l = 1$ (or equivalently when summing up the equations over j and l , as in [4]) we obtain :

$$0 = \int_{\Omega_h} (u_h^{n+1,-} - u_h^{n,-}) + \int_{t^n}^{t^{n+1}} \sum_{i=0}^N \int_{x_i}^{x_{i+1}} \partial_x f_h(u_h) = \int_{\Omega_h} (u_h^{n+1,-} - u_h^{n,-}) + \int_{t^n}^{t^{n+1}} (\hat{f}_h(u_h) |_{x=L} - \hat{f}_h(u_h) |_{x=0})$$

having introduced the numerical fluxes associated to the boundary conditions $\hat{f}_h(u_h) |_{x=0}$, and $\hat{f}_h(u_h) |_{x=L}$. Summing up over n we finally obtain the global

conservation statement :

$$0 = \int_{\Omega_h} (u_h(x, T^-) - u_h(x, 0)) + \int_0^T (\hat{f}_h(u_h)|_{x=L} - \hat{f}_h(u_h)|_{x=0})$$

Note that under similar conditions a Lax-Wendroff theorem can be proved: when converging (with respect to h and Δt) the scheme converges to a weak solution of (1). We refer to [4, 9] for details.

Before discussing the definition of the test functions, we are left with one degree of freedom, namely the definition of the continuous $f_h(u_h)$, or equivalently of the discrete divergence $\partial_x f_h(u_h)|_{K_i^n}$. To do this, we are aided by the following simple result.

Proposition 2.1 (Trapped steady shocks). *If the same continuous approximation is used for f_h and u_h , scheme (8) admits a spurious solution consisting of (at least one) steady state shock trapped in a single cell $[i, i + 1]$.*

Proof. Consider the initial solution $u_i = u_L$ if $x_i \leq x_{\text{shock}}$ and $u_i = u_R$ otherwise. Across steady shocks we know that $[f] = f(u_R) - f(u_L) = 0$. Set $f(u_R) = f(u_L) = f_0$. Trivially, scheme (8) admits the steady solution $u_h = u_h(x, 0)$, since for this choice we have identically $\partial_t u_h|_K = \partial_x f_h|_K = 0$, since for this solution

$$f_h|_{K_i^n} = \sum_{j=1}^{k+1} \sum_{l=1}^{m+1} \varphi_j^s(x) \varphi_l^t(t) f_0 = f_0$$

□

For this reason, we have chosen to use in all numerical computations the discrete flux

$$f_h|_{K_i^n} = \sum_{\sigma=1}^{k+2} \sum_{l=1}^{m+1} \bar{\varphi}_\sigma^s(x) \varphi_l^t(t) f(u_\sigma^l), \quad u_\sigma^l = \sum_{j=1}^{k+1} \varphi_j^s(x_\sigma) u_j^l \quad (9)$$

having denote by $\bar{\varphi}_\sigma^s$ the $(k + 1)$ degree Lagrange polynomial basis functions in space, and with $\{x_\sigma\}_{\sigma=1}^{k+2}$ the corresponding (equally spaced) interpolation points in K . The extra reconstructed interpolation point allows to break spurious steady shocks.

3 Properties of the discretization

3.1 Accuracy conditions

We extend the consistency analysis of [3, 27, 4, 5] to (8). In Appendix A we prove the following result.

Proposition 3.1 (Consistency estimate). *Consider a smooth compactly supported function $\psi \in C_0^{r+1}([0, L] \times [0, T])$, with $r \geq \max(k, m)$, and an exact*

smooth solution of (1), $u \in H^{r+1}([0, L] \times [0, T])$. Define the truncation error

$$e(\psi, h, \Delta t) = \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \sum_{j=1}^{k+1} \sum_{l=1}^{m+1} \psi_j^l \left\{ \int_{K_i^n} \beta_j^l(x, t) (\partial_t u_h + \partial_x f_h(u_h)) + \int_{\Omega_h \cap K_i^n} \beta_j^l(x, t^{n,+}) [u_h(x)]^n \right\} \quad (10)$$

having denoted by ψ_j^l the nodal values corresponding to the L^2 projection of ψ onto the approximation space, the pairs $\{(x_j, t^l)\}_{j=1, k+1}^{l=1, m+1}$ representing the grid of degrees of freedom on K_i^n , and with u_h the approximation (5) of the exact solution u . Let the space-time grid verify

$$\nu_0 \leq \frac{\Delta t}{h} \leq \nu_1, \quad 0 < \nu_0, \nu_1 < \infty \quad (11)$$

Let also

$$\|\psi_h\|_{L^\infty} \leq \|\psi\|_{L^\infty} \leq C_1, \quad \|\partial_t \psi_h\|_{L^\infty} \leq \|\partial_t \psi\|_{L^\infty} \leq C_2, \quad \|\partial_x \psi_h\|_{L^\infty} \leq \|\partial_x \psi\|_{L^\infty} \leq C_3 \quad (12)$$

for some positive constants C_1 , C_2 , and C_3 , and in particular

$$\sup_{j, \sigma, l, r} |\psi_j^l - \psi_\sigma^r| \leq \max(C_2, C_3) h \quad (13)$$

Under these hypotheses, scheme (8) verifies the truncation error estimate

$$|e(\psi, h, \Delta t)| \leq C h^p, \quad p = \min(k+1, m+1) \quad (14)$$

provided that the spatial and temporal approximations u_h and f_h respectively are p th order accurate.

While details of the proof are reported in Appendix A, for the following discussion, we remark that the error can be recast easily as

$$\begin{aligned} e(\psi, h, \Delta t) = & - \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \left\{ \int_{K_i^n} (u_h \partial_t \psi_h + f_h(u_h) \partial_x \psi_h) + \int_{K_i} [\psi_h]^{n+1} \hat{u}_h^{n+1} - \int_{K_i} [\psi_h]^n \hat{u}_h^n \right\} + \\ & \frac{1}{(k+1)(m+1)} \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i^n} (\beta_j^l(x, t) - \varphi_j^s(x) \varphi_l^t(t)) (\partial_t u_h + \partial_x f_h(u_h)) + \\ & \frac{1}{(k+1)(m+1)} \sum_{n=0}^M \sum_{K_i} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i} (\beta_j^l(x, t^{n,+}) - \varphi_j^s(x) \varphi_l^t(t^{n,+})) [u_h]^n \end{aligned} \quad (15)$$

which shows the contributions of both volume and trace terms.

3.2 Positivity

For scalar problems, the theory of positive coefficient schemes [31] allows to characterize variations in space and time of the discrete solution, and to ensure that a discrete maximum principle is observed. For scheme (8), we have the following characterization.

Proposition 3.2 (Discrete maximum principle). *Provided that*

$$\int_{K_i^n} \beta_j^l(x, t) (\partial_t u_h + \partial_x f_h(u_h)) = \sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} c_{j\sigma}^{lr} (u_j^l - u_\sigma^r) \quad \text{with } c_{j\sigma}^{lr} \geq 0$$

$$\int_{K_i} \beta_j^l(x, t^{n,+}) [u_h(x)]^n = \sum_{\sigma=1}^{k+1} c_{j\sigma}^{l,-} (u_j^l - u_\sigma^{n,-}) \quad \text{with } c_{j\sigma}^{l,-} > 0 \text{ for at least one triplet } (j, \sigma, l)$$
(16)

then the solution of scheme (8) verifies the discrete inequality

$$u_-^n = \min_{\sigma \in \Omega_h} u_\sigma(t^{n,-}) \leq u_j(t^{n,+}), \{u_j^l\}_{2 \leq l \leq m}, u_j(t^{n+1,-}) \leq \max_{\sigma \in \Omega_h} u_\sigma(t^{n,-}) = U_+^n \quad \forall j \in \Omega_h$$
(17)

The proof of the proposition is reported in Appendix B. Schemes preserving the positivity of the unknown and respecting the discrete maximum principle (17) independently on the time step can be constructed provided that we are able to retain conditions (16) in practice.

3.3 Choice of the trace

We introduce here a first simplification of the discrete prototype (8). As the error analysis shows (cf. section §3.1 and appendix A), the necessary conditions for the scheme to verify the error estimate (14) is that the test functions and the traces of the test functions on the lower boundary are to be uniformly bounded w.r.t space and time step, and solution data. A particular simple choice of the traces is suggested by the last term in the truncation error (15). In the following, we shall assume that we can find test functions $\beta_j^l(x, t)$ such that

$$\lim_{t \rightarrow t^{n,+}} \beta_j^l(x, t) = \varphi_j^s(x) \varphi_i^t(t^{n,+}), \quad \forall i, l$$
(18)

This would correspond to a form of *bubble stabilized* Galerkin formulation, which, for the approximation choice made here, can be written as

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^l(x, t) (\partial_t u_h + \partial_x f_h(u_h)) = 0, \quad \text{for } u_j^l \text{ with } j \in \Omega_h \text{ and } 2 \leq l \leq m+1$$

$$\int_{t^n}^{t^{n+1}} \int_{\Omega_h} \beta_j^{n,+}(x, t) (\partial_t u_h + \partial_x f_h(u_h)) + \int_{\Omega_h} \varphi_j^s(x) [u_h(x)]^n = 0, \quad \text{for } u_j^{n,+} \text{ with } j \in \Omega_h$$
(19)

In this case, the last term in the error representation (15) vanishes identically.

4 Numerical quadrature and examples of schemes

In the following section, we discuss numerical results obtained on linear and nonlinear problems for approximations $P^k P^m$ with $k, m \in \{1, 2, 3\}$, and with

different definitions of the test functions β_j^l in (19). Before describing the choice of these functions we consider the fully discrete version of (19) obtained by replacing the continuous integrals by tensor product approximate quadrature forms :

$$\begin{aligned} \sum_{K_i^n | j \in K_i} \sum_{p_s=1}^{Q_s} \sum_{p_t=1}^{Q_t} \omega_{p_s} \omega^{p_t} \beta_j^l(x_{p_s}, t^{p_t}) (\partial_t u_h + \partial_x f_h(u_h))(x_{p_s}, t^{p_t}) &= 0, \quad 2 \leq l \leq m+1 \\ \sum_{K_i^n | j \in K_i} \sum_{p_s=1}^{Q_s} \sum_{p_t=1}^{Q_t} \omega_{p_s} \omega^{p_t} \beta_j^{n,+}(x_{p_s}, t^{p_t}) (\partial_t u_h + \partial_x f_h(u_h))(x_{p_s}, t^{p_t}) \\ &+ \sum_{K_i | j \in K_i} \sum_{p_s=1}^{Q_s} \omega_{p_s} \varphi_j^s(x_{p_s}) [u_h(x_{p_s})]^n = 0 \end{aligned}$$

where the discrete approximations u_h and $f_h(u_h)$ are obtained by means of (5) and (9), respectively. The question is now how to choose the quadrature formulas. The criterion used here is that each equations should correspond to a splitting of the *exact integral* of the discrete space time divergence, in other words that when summing up all the equations over a space time element K_i^n we should obtain the exact integral of $\partial_t u_h + \partial_x f_h$. In formulas, we want the identity

$$\sum_{p_s=1}^{Q_s} \sum_{p_t=1}^{Q_t} \omega_{p_s} \omega^{p_t} (\partial_t u_h + \partial_x f_h(u_h))(x_{p_s}, t^{p_t}) + \sum_{p_s=1}^{Q_s} \omega_{p_s} [u_h(x_{p_s})]^n = \int_{K_i^n} (\partial_t u_h + \partial_x f_h(u_h))_{K_i^n} + \int_{K_i} [u_h(x)]_{K_i}^n$$

to hold exactly. For approximations (5) and (9), this requires the one-dimensional formulas used in the tensor product quadrature to be exact for polynomials of degree k in space and m in time, thus allowing the use of the formulas naturally defined by the one-dimensional elements. This further simplifies the form of the scheme. Indeed, due to the interpolation properties $\varphi_j^s(x_\sigma) = \delta_{j\sigma}$ and $\varphi_l^t(t^r) = \delta_{lr}$ we obtain the fully discrete form used in the calculations

$$\begin{aligned} \sum_{K_i^n | j \in K_i^n} \sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} \omega_\sigma \omega^r \beta_j^l(x_\sigma, t^r) (\partial_t u_\sigma(t^r) \delta_{j\sigma} + \partial_x f_h(x_\sigma, t^r)) &= 0 \quad 2 \leq l \leq m+1 \\ \sum_{K_i^n | j \in K_i^n} \sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} \omega_\sigma \omega^r \beta_j^{n,+}(x_\sigma, t^r) (\partial_t u_\sigma(t^r) \delta_{j\sigma} + \partial_x f_h(x_\sigma, t^r)) &+ \Delta x_j [u_j]^n = 0 \end{aligned}$$

where

$$\Delta x_j = \sum_{K_i | j \in K_i} \omega_j (x_{i+1} - x_i)$$

It only remains to define the test functions β_j^l in space-time elements.

4.1 Space-time GLS($P^n P^m$)

In order to test our formulation and verify our code, we consider the Galerkin-Least-Squares scheme. In particular, let

$$\kappa_j^l(x, t) = \varphi_j^s(x) \frac{d\varphi_l^t(t)}{dt} + \frac{d\varphi_j^s(x)}{dx} \varphi_l^t(t), \quad (20)$$

the GLS scheme is obtained by setting in (19) (cf. [6] and references therein)

$$\beta_j^l(x, t) = \varphi_j^s(x) \varphi_l^t(t) + \kappa_j^l(x, t) \tau(x, t), \quad \tau(x, t) = 2 \left(\sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} |\kappa_\sigma^r(x, t)| \right)^{-1} \quad (21)$$

The GLS scheme verifies the consistency estimate of proposition 3.1, and can be shown to be energy stable, and to actually converge to weak solutions of (1). The interested reader is referred to [24, 23, 32, 25, 18, 6] and references therein for more.

4.2 Space-time LDA($P^n P^m$)

We consider the Petrov-Galerkin space-time formulation of the so-called multi-dimensional upwind LDA residual distribution scheme [15, 34]. This formulation is obtained on the space time element K_i^n by applying the residual distribution philosophy to the non-integrated residual (constant advection case) :

$$\phi_h = (\partial_t u_h + a \partial_x u_h)_{K_i^n} = \sum_{j=1}^{k+1} \sum_{l=1}^{m+1} \kappa_j^l(x, t) u_j^l$$

with κ_j^l given by (20). The LDA residual distribution is obtained by assigning to the degree of freedom corresponding to u_j^l the split residual

$$\phi_j^l = \max(0, \kappa_j^l) \left(\sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} \max(0, \kappa_\sigma^r) \right)^{-1} \phi_h$$

Conservative equations are obtained now by integrating these local contributions over the element, leading to the sought Petrov-Galerkin form. In our case, this leads to the use of

$$\beta_j^l(x, t) = \max(0, \kappa_j^l) \left(\sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} \max(0, \kappa_\sigma^r) \right)^{-1} \quad (22)$$

in (19), with κ_j^l as in (20). The interested reader is referred to [15, 34] for more. We will refer to this discretization as to the LDA scheme, even though, technically speaking, it is not anymore a residual distribution scheme. The LDA scheme verifies the consistency estimate of proposition 3.1.

4.3 Space-time LLFs($P^n P^m$)

We construct a positivity preserving scheme based on the Limited and Stabilized Lax Friedrich's discretization of [1, 28, 2]. The principle is to start from a first order scheme that verifies the first of (16). In our case, this is obtained by defining on each K_i^n the quantity

$$\Phi_j^l = \frac{1}{(k+1)(m+1)} \int_{K_i^n} \overbrace{(\partial_t u_h + \partial_x f_h)}^{\Phi_h} + \frac{\alpha}{(k+1)(m+1)} \sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} (u_j^l - u_\sigma^r) \quad (23)$$

with the condition

$$\alpha > \max(h, \Delta t) \max_{(x,t) \in K_i^n} \|(1, \partial_u f(u_h))\|_{L^\infty}$$

guaranteeing that the first in (16) is verified. The next step is to compute uniformly bounded *distribution coefficients* as [1, 2]

$$\gamma_j^l = \frac{\max(0, \Phi_j^l \Phi_h)}{\sum_{\sigma=1}^{k+1} \sum_{r=1}^{m+1} \max(0, \Phi_\sigma^r \Phi_h)}$$

with Φ_h implicitly defined in (23). Note that one easily shows that

$$\gamma_j^l \Phi_h = \nu_j^l \Phi_j^l, \quad \nu_j^l \in [0, 1] \quad (24)$$

Lastly, we evaluate (19), setting in each space-time element K_i^n

$$\beta_j^l(x, t) = \gamma_j^l + \delta_0(u_h) \delta_1(u_h) \kappa_j^l(x, t) \tau(x, t) \quad (25)$$

with κ_j^l as in (20) and τ as in (21). The scheme obtained in this way is referred to as the LLFs scheme. For $\delta_0 \delta_1 = 0$ we obtain $\beta_j^l = \gamma_j^l$. In this case we refer to the scheme as to the LLF (limited Lax-Friedrich's). Note that, due to (24), the LLF scheme is easily shown to verify proposition 3.2. However, as shown in [1, 28, 2], the extra term is necessary to achieve to convergence rates of proposition 3.1. The objective of the δ_0 and δ_1 sensors is to recover the properties of the LLF scheme where needed.

In particular, the quantity $\delta_1(u_h)$ is a smoothness sensor which is defined following [1, 28] as

$$\delta_1(u_h) = \min \left(1, \frac{\|u_h\|_{L^\infty(K_i^n)} \|\partial_x f(u_h)\|_{L^\infty(K_i^n)}}{|\partial_t u_h + \partial_x f_h(u_h)|} \right)$$

note that δ_1 is a function of (x, t) , evaluated in each quadrature point when evaluating (19). The scope of δ_1 is to recover the non-oscillatory character of the LLF scheme across discontinuities.

The function $\delta_0(u_h)$ is instead a *positivity sensor*. We use an improved version of the one proposed in [28]. In particular we set

$$\delta_0 = \frac{1}{2} \left(1 + \tanh \left(\alpha \tan \left(\pi * \left(0.5 - e^{-\frac{c^* u_{min}}{U_{max}^n - u_{min}}} \right) \right) \right) \right)$$

where U_{max}^n is the maximal (necessarily positive) value of the considered component over the whole solution between time steps n and $n + 1$

$$U_{max}^n = \max_{i \in \Omega_h, 1 \leq l \leq m+1} u_j^l,$$

u_{min} is the local minimal value within the considered space-time element K_i^n

$$u_{min} = \min_{(j,l) \in K_i^n} u_j^l,$$

and c is a cut-off parameter such that the exponential takes the value 0.5 when u_{min} equals a cut-off value ξ . A short calculation gives:

$$c = \ln(2) \frac{\mathbf{u}_{max}^n - \xi}{\xi}.$$

Finally, α is a parameter tuning the steepness of the hyperbolic tangent around the cut-off value. During our computations, we have been using the following values:

$$\alpha = 1.0, \quad \xi = \left(\frac{dx}{k} \frac{dt}{m} \right)^2.$$

The use of δ_0 allows, for component of the solution under a strict positivity constraint, to recover the positivity preserving property of the LLF scheme, in particular the preservation of the non-negativity of the solution, consequence of the left inequality in (17).

Appendix A : proof of proposition 3.1

We report here the proof of proposition 3.1. We start by remarking that using the consistency condition (7) and the interpolation property

$$\sum_{j=1}^{k+1} \sum_{l=1}^{m+1} \varphi_j^s \varphi_l^t = 1$$

by simple manipulations one can recast the error as

$$\begin{aligned} e(\psi, h, \Delta t) = & - \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \left\{ \int_{K_i^n} (u_h \partial_t \psi_h + f_h(u_h) \partial_x \psi_h) + \int_{K_i} [\psi_h]^{n+1} \hat{u}_h^{n+1} - \int_{K_i} [\psi_h]^n \hat{u}_h^n \right\} + \\ & \frac{1}{(k+1)(m+1)} \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i^n} (\beta_j^l(x, t) - \varphi_j^s(x) \varphi_l^t(t)) (\partial_t u_h + \partial_x f_h(u_h)) + \\ & \frac{1}{(k+1)(m+1)} \sum_{n=0}^M \sum_{K_i} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i} (\beta_j^l(x, t^{n,+}) - \varphi_j^s(x) \varphi_l^t(t^{n,+})) [u_h]^n \end{aligned} \tag{26}$$

By simple arguments, one can also show that the exact solution verifies

$$- \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \left\{ \int_{K_i^n} (u \partial_t \psi_h + f(u) \partial_x \psi_h) + \int_{K_i} [\psi_h]^{n+1} u^{n+1} - \int_{K_i} [\psi_h]^n u^n \right\} = 0$$

So that the error can be recast as

$$e(\psi, h, \Delta t) = \text{I} + \text{II} + \text{III} + \text{IV}$$

with

$$\begin{aligned}
\text{I} &= - \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \int_{K_i^n} ((u_h - u) \partial_t \psi_h + (f_h(u_h) - f(u)) \partial_x \psi_h) \\
\text{II} &= \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \int_{K_i^n} [\psi_h]^{n+1} (\hat{u}_h^{n+1} - u^{n+1}) - \int_{K_i^n} [\psi_h]^n (\hat{u}_h^n - u^n) \\
\text{III} &= \frac{1}{C_{K_i^n}} \sum_{K_i^n \in \Omega_h \times \mathcal{T}_{\Delta t}} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i^n} (\beta_j^l(x, t) - \varphi_j^s(x) \varphi_l^t(t)) (\partial_t (u_h - u) + \partial_x (f_h(u_h) - f(u))) \\
\text{IV} &= \frac{1}{C_{K_i^n}} \sum_{n=0}^M \sum_{K_i^n} \sum_{\sigma, j=1}^{k+1} \sum_{r, l=1}^{m+1} (\psi_j^l - \psi_\sigma^r) \int_{K_i^n} (\beta_j^l(x, t^{n,+}) - \varphi_j^s(x) \varphi_l^t(t^{n,+})) ((u_h^{n,+} - u^n) - (u_h^{n,-} - u^n))
\end{aligned}$$

with $C_{K_i^n} = (k+1)(m+1)$. We can now estimate the magnitude of the error by bounding all the terms on the right hand side.

Using classical approximation results [11, 17] and (11) we can argue that

$$|u_h - u|, |f_h - f| = \mathcal{O}(h^p) \quad \text{and} \quad |\partial_t(u_h - u)|, |\partial_x(f_h - f)| = \mathcal{O}(h^{p-1}) \quad (27)$$

Thanks to (12) we immediately deduce that

$$|\text{I}| \leq C'_a(\Omega_h, \mathcal{T}_{\Delta t}) h^{-2} h^2 h^p \leq C_a(\Omega_h, \mathcal{T}_{\Delta t}) h^p$$

having used the fact that the total number of space-time elements is of the order $(h \Delta t)^{-1}$ and (11). Similarly, using (13), the boundedness of β_j^l and of the basis functions $\varphi_j^s \varphi_l^t$, and (27) we deduce

$$|\text{III}| \leq C'_b(\Omega_h, \mathcal{T}_{\Delta t}) h^{-2} h h^2 h^{p-1} \leq C_b(\Omega_h, \mathcal{T}_{\Delta t}) h^p$$

Term IV is also easily estimated, since for both projections $u_h^{n,\pm}$ we have [11] $|u_h^{n,\pm} - u^n| = \mathcal{O}(h^p)$, hence

$$|\text{IV}| \leq C'_c(\Omega_h, \mathcal{T}_{\Delta t}) h^{-2} h h^2 h^p \leq C_c(\Omega_h, \mathcal{T}_{\Delta t}) h^{p+1}$$

Lastly, using the Lipschitz continuity and the consistency of the numerical fluxes \hat{u}_h in term II we can write

$$\begin{aligned}
|\hat{u}_h^n - u^n| &\leq |\hat{u}_h^n(u_h^{n,+}, u_h^{n,-}) - u_h^{n,+}| + |u_h^{n,+} - u^n| \leq L_{\hat{u}} |[u_h]^n| + C'_d h^p \\
&\leq L_{\hat{u}} |u_h^{n,+} - u^n| + L_{\hat{u}} |u_h^{n,-} - u^n| + C'_d h^p \leq L_{\hat{u}} C''_d h^p + L_{\hat{u}} C''_d h^p + C'_d h^p
\end{aligned}$$

Moreover, for the jumps in ψ_h we can also write

$$|[\psi_h]^n| = |\psi_h^{n,+} - \psi^n + \psi^n - \psi_h^{n,-}| \leq |\psi_h^{n,+} - \psi^n| + |\psi^n - \psi_h^{n,-}| \leq C h^p$$

leading to

$$|\text{II}| \leq C_d(\Omega_h, \mathcal{T}_{\Delta t}) h^{-2} h^2 h^p h^p = C_d(\Omega_h, \mathcal{T}_{\Delta t}) h^{2p}$$

which achieves the proof.

Appendix B : proof of proposition 3.2

In order to prove proposition 3.2 we start by rewriting (8) as

$$CU = b^-$$

with C a square $(N + 1) \times (m + 1)$ matrix with

$$C_{\alpha_{jl}\beta_{\sigma r}} = \sum_{K_i^n | u_\sigma^l, u_\sigma^r \in K_i^n} c_{j\sigma}^{lr} \Big|_{K_i^n} + \sum_{K_i^n | u_\sigma^l \in K_i^n, u_\sigma^{n,-} \in K_i} c_{j\sigma}^{l,-} \Big|_{K_i^n}$$

$\alpha_{jl} = j l, \beta_{\sigma r} = \sigma r$ with $j, \sigma = 1, N + 1$ and $l, r = 1, m + 1$

and with

$$b^- = C^- U^-$$

where U is the $(N + 1)(m + 1)$ array of unknowns, U^- is the $N + 1$ array containing the values $u_\sigma^{n,-}$, C^- is a $(N + 1)(m + 1) \times (N + 1)$ rectangular matrix with

$$C_{\alpha_{jl}\sigma}^- = \sum_{K_i^n | u_\sigma^l \in K_i^n, u_\sigma^{n,-} \in K_i} c_{j\sigma}^{l,-} \Big|_{K_i^n}$$

and noting that by hypothesis

- C is an L-matrix ($C_{\alpha_{jl}\alpha_{jl}} \geq 0, C_{\alpha_{jl}\beta_{\sigma r}} \leq 0$) ;
- C is irreducibly diagonally dominant. In particular, for the rows corresponding to the triplets (j, σ, l) verifying the second hypothesis in (16) we have

$$\begin{aligned} |C_{\alpha_{jl}\alpha_{jl}}| - \sum_{\sigma, r} |C_{\alpha_{jl}\beta_{\sigma r}}| &= \sum_{K_i^n | u_\sigma^l, u_\sigma^r \in K_i^n} c_{j\sigma}^{lr} \Big|_{K_i^n} + \sum_{K_i^n | u_\sigma^l \in K_i^n, u_\sigma^{n,-} \in K_i} c_{j\sigma}^{l,-} \Big|_{K_i^n} - \sum_{K_i^n | u_\sigma^l, u_\sigma^r \in K_i^n} c_{j\sigma}^{lr} \Big|_{K_i^n} \\ &= \sum_{K_i^n | u_\sigma^l \in K_i^n, u_\sigma^{n,-} \in K_i} c_{j\sigma}^{l,-} \Big|_{K_i^n} > 0 \end{aligned}$$

Hence, C is an irreducibly diagonally dominant L-matrix, and its inverse is positive [7] : $C_{j\sigma}^{-1} \geq 0 \forall j \sigma$. Not also that

$$C\bar{\mathbf{1}} = C^- \mathbf{1} = r^-, \quad r_{\alpha_{jl}}^- = \sum_{K_i^n | u_\sigma^l \in K_i^n, u_\sigma^{n,-} \in K_i} c_{j\sigma}^{l,-} \Big|_{K_i^n} > 0 \quad (28)$$

where $\alpha_{jl} = j l, \beta_{\sigma r} = \sigma r$ with $j = 1, N + 1$ and $l = 1, m + 1$, and with $\bar{\mathbf{1}}$ and $\mathbf{1}$ the $(N + 1)(m + 1)$ and $N + 1$ arrays of ones. Finally (equalities/inequalities meant by component)

$$CU = C^- U^- \stackrel{C_{j\sigma}^- \geq 0}{\geq} C^- \mathbf{1} u_-^n \stackrel{\text{eq. (28)}}{=} C\bar{\mathbf{1}} u_-^n$$

The left inequality is obtained upon multiplication by the positive matrix C^{-1} . Similarly one obtains the right inequality.

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