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ON HIGH RESOLUTION VARIANTS OF LAGRANGE–GALERKIN FINITE–ELEMENT SCHEMES

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VARIANTES A HAUTE RESOLUTION DE QUELQUES SCHEMAS AUX ELEMENTS FINIS LAGRANGE–GALERKIN

Résumé :

Nous étudions comment des schémas monodimensionnel en volumes finis à haute résolution (des discontinuités) comme FCT ou MUSCL peuvent être introduits dans un contexte multidimensionnel d'éléments finis Lagrange–Galerkin.

ON HIGH RESOLUTION VARIANTS OF LAGRANGE–GALERKIN FINITE–ELEMENT SCHEMES

Abstract :

It is shown how two typical 1D finite–volume high resolution schemes, like FCT or MUSCL can be introduced in the multidimensional background of a class of Lagrange–Galerkin finite–element methods.

This short note is devoted to a set of ideas starting from the fact that (??) high resolution finite volume methods are more or less the best methods for some class of 1D problems while (??) Lagrange-Galerkin finite element methods are thought to be among the best ones for taking into account non structured meshes.

Our point of view is that many qualities of both approaches can be rationally combined, providing a numerical method that can be enriched in a compatible manner by both finite volume or finite element discretized extra terms such as diffusion terms. This should give a better understanding of the derivation of several existing schemes for which numerical experiments are available (see [2], [3-8, 21], [10], [11]) for upwind schemes and [14, 22] for FCT schemes and in the other references given in the text.

1 Mathematical models

We shall consider 2D situations for the sake of simplicity but most of the ideas presented in this note can be extended to 3D.

We are interested by schemes that apply to a class of Partial Differential Equations involving, as in compressible CFD for instance, hyperbolic terms and parabolic (diffusion) terms. We shall in fact restrict ourselves to the following models :

$$\text{Advection model} \ : \ u_t + \vec{V} \ . \ \vec{grad} \ u = 0, \ u \epsilon \ I\!R^d, \ d = 1 \tag{1}$$

$$\text{Conservation law} \ : \ u_t + \ div \ (\vec{V} u) = 0, \ u \epsilon \ I\!R^d, \ d = 1 \tag{2}$$

$$\text{Hyperbolic system} \ : \ w_t + \ div \ \vec{\mathcal{F}}(w) = 0, \ u \epsilon \ I\!R^d, \ d \geq 1 \tag{3}$$

in which u is a scalar unknown, w a vector, $\vec{V}$ a given vector field assumed to be divergence free (so that (??) is a particular case of (??)), and $\vec{\mathcal{F}}$ a hyperbolic flux vector with a Jacobian $\mathcal{A} = \frac{\partial \mathcal{F}}{\partial w}$ diagonalizable in any direction. Parabolic variants of (??) and (??) are written

$$u_t + \vec{V} \ . \ \vec{grad} \ u - \Delta u = 0 \tag{4}$$

$$u_t + \ div \ (\vec{V} u) - \Delta u = 0 \tag{5}$$

Boundary conditions - a wide and interesting question - will not be discussed in this note.

2 Lagrange-Galerkin formulation

Let $\mathcal{T}$ be a triangulation of $I\!R^2$ in finite elements. Let V_h^d be a set of functions from $I\!R^2$ with values in $I\!R^d$ that are continuous , and equal on each element to a polynomial with degree $\leq k$. Further, the basis of V_h is a set at functions ϕ_j satisfying the following Lagrange interpolation conditions :

* There exists a set of nodes $\vec{x}_j \ for \ j = 1, \ \cdots, \ N$

* To each node $\vec{x}_j$ there corresponds exactly one basis function ϕ_j

* $\phi_j = \delta_{jk}$ on x_k (Kronecker)

We shall consider the following abstract family of schemes :

$$\int W_t \phi \ dv \ + \int \ \phi \ div \ \mathcal{F}(W) \ dv \ + \epsilon_d \int \nabla \phi \nabla W \ dv = 0 \tag{6}$$

($\epsilon_d = 0$ for $d > 1$) in which $\mathcal{F}(w)$ is considered as an element of V_h^d ; the spatial scheme is described ; for the temporal derivative one possibility is to apply a linearized version of the Runge–Kutta scheme introduced by A. Jameson [15] :

$w^{(0)} = \omega^n$, for $l = 0, \ k-1$, for any $\phi \in V_h^d$, find $W^{(l+1)}$ in V_h^d such that :

$$\int \frac{w^{(l+1)} - \omega^{(0)}}{\alpha_k \Delta t} \phi d\sigma + \int \phi \ div \ \mathcal{F}_{(\omega}^{(l)} + \epsilon_d \int \nabla \phi \nabla w^{(l)} = 0 \tag{7}$$

For $k = 1$ this schemes reduces to the Euler forward but it is not explicit due to the fact that Lagrange-Galerkin mass matrix is not diagonal. However, a mass–lumped variant can prove to be interesting : it is written

$$d_i \frac{W_i^{(k+1)}}{\alpha_k \Delta t} - W_i^{(0)} + \int \phi_i \ div \ \mathcal{F}_{(w)}^{(l)} + \epsilon_d \int \nabla \phi_i \nabla_w^{(l)} = 0 \tag{8}$$

For stability a CFL condition can generally be found by Fourier Analysis for structured meshes.

Schemes (??) and (??) have been tried by many authors for P_1 or Q_1 elements ; a very short P_2 experiment is also presented in [12].

3 First order Godunov variant

The robustness of an approximation of (??)-(??) can be measured at two level :

level 1 : The maximum principle is satisfied for (??), and positiveness preservation for (??).

level 2 : No oscillation, or only a few oscillations, can occur.

We are interested in this section to level 1, which is necessary for a safe simulation of complex flows in which, for example, species concentrations must be kept between 0 and 1.

Clearly (except under some condition between the mesh size and the Peclet number) the Lagrange–Galerkin methods are not of level 1 or 2. We now try now to add to them the right amount of upwinding (robustness of parabolic terms is not addressed).

We remark first that Lagrange–Galerkin methods are finite–volume schemes in some extended sense ; indeed the divergence operator can be written :

$$(\mathcal{M}\mathcal{F})_i = \sum_j \int F_j \phi_i \; div \; \vec{\phi}_j \; dv = \sum_j \mathcal{M}_{ij} \; . \; F_j \tag{9}$$

with $\vec{\phi}_j =^t (\phi_j, \phi_j)$. Since $\mathcal{M}$ is antisymmetric, we have

$$\mathcal{M}_{ii} = 0 \; \forall_i$$

and constant vectors belong to its kernel so that

$$\sum_j \mathcal{M}_{ij} = 0 \; \forall_i$$

So that

$$\sum_j \mathcal{M}_{ij} \; \mathcal{F}_j = \sum_{j \neq i} 2 \; \mathcal{M}_{ij} \; . \; \frac{\mathcal{F}_i + \mathcal{F}_j}{2} \tag{10}$$

The right-hand side is a finite-volume flux integration between node i and node j with the following mean normal vector (elementory flux) :

$$\begin{aligned} \eta_{ij}^x &= \; 2 \int \phi_i \frac{\partial \phi_j}{\partial x} \; dv \\ \eta_{ij}^y &= \; 2 \int \phi_i \frac{\partial \phi_j}{\partial y} \; dv \end{aligned} \tag{11}$$

Further we recognize a central-differenced integration since a pure arithmetic mean is taken between $\mathcal{F}_i$ and $\mathcal{F}_j$; let us write in the above scheme :

$$\mathcal{MF} = \sum_{j \neq i} \Phi^{central}(W_i, W_j, \eta_{ij}) \tag{12}$$

In the particular case of a P_1 method, it has been observed [6, 7, 8] that η_{ij} is the integration of the normal vector between neighbour cells if these cells are delimited by element-medians (Figure 1).

$$\vec{\eta}_{ij} = \int_{\partial\ C_i \cap \partial\ C_j} \vec{\eta}\ d\sigma = 2 \int \int \phi_i \vec{\nabla} \phi_j\ dv \tag{13}$$

Figure 1 : Elementary fluxes in P1 case.
(cell boundaries are medians!)

Instead of applying a central differenced integration, we can consider the evolution of a Riemann problem with W_i and W_j as left and right states and $\vec{\eta}_{ij}$ for defining the interface (normal to $\vec{\eta}_{ij}$).
Then a Godunov extension of the Lagrange–Galerkin scheme can be defined from :

$$\mathcal{M}^{Godunov}(F) = \sum_{j \neq i} \Phi^{Riemann}(W_i, W_j, \eta_{ij}) \tag{14}$$

in which the flux $\Phi^{Riemann}$ is derived from the solution $\vec{W}(\frac{x}{t})$ of the Riemann problem, for example by taking its value at $\frac{x}{t} = 0$:

$$\Phi^{Riemann}(W_i, W_j, \eta_{ij}) = \vec{\mathcal{F}}(\bar{W}(0))\ .\ \vec{\eta}_{ij} \tag{15}$$

Another possibility is to apply an Approximate Riemann Solver like Roe's Solver :

$$\Phi^{Roe}(W_i, W_j, \vec{\eta}_{ij}) = \frac{\mathcal{F}(W_i) + \mathcal{F}(W_j)}{2}\ .\ \vec{\eta}_{ij} + \frac{1}{2}|\mathcal{A}\eta_{ij}|(W_j - W_i) \tag{16}$$

(See [16] for details).

In the case of (??) or (??), $\mathcal{A}$ reduces to $\vec{V}\ .\ \vec{\eta}_{ij}$ and we obtain an extension of the donor cell scheme

$$\Phi^{Donor}(W_i, W_j,\ \vec{\eta}_{ij}) = \frac{V_i + V_j}{2}\ .\ \eta_{ij}(u_i + u_i) + \frac{1}{2}|V_i + V_j)\ .\ \eta_{ij}|(u_j - u_i)$$

Lemma 1 : *In the case of model 2, the whole family of upwind Lagrange–Galerkin schemes satisfies the posivity preservation when advanced with the mass–lumped RK*1 *scheme, under the following CFL condition (case* $\epsilon_1 = 0$*, l no parabolic terms) :*

$$d_i - \Delta t \sum_j \vec{V}_{ij}\ .\ \vec{\eta}_{ij} \geq 0 \tag{17}$$

Remark 1 : The maximum principle can also be obtained for passive species by combining with the formulation presented in [9].

Remark 2 : The Q_1 case : Q_1 Lagrange approximations are richer in interpolation and can degenerate easily from 3D to 2D and from 2D to 1D (solutions are identical). For this case we note that η_{ij} does not rely any more on a tessellation. In particular, beside edges, diagonal of quadrilateral also support flux integration

Figure 2 : flux integration around a node i for a quadrilateral mesh.

4 FCT variant

One way to construct a high (discontinuity) resolution scheme is to apply Zalesak's FCT construction [13] for coupling the first–order accurate Godunov scheme of Section 3 with the higher–order central–differenced scheme of Section 4. This is rather easy since both schemes are finally assembled by a flux accumulation of the following form.

$$d_i W_i^{n+1} = d_i W_i^n + \sum_{j \neq i} \Phi_{ij} \tag{18}$$

With for the low–order scheme

$$\Phi_{ij}^{low} = \Phi^{Roe}(W_i, W_j, \vec{\eta}_{ij}) \tag{19}$$

and for the high–order scheme :

$$\Phi_{ij}^{high} = \Phi^{central}(W_i^{(k-1)}, W_j^{(k-1)}, \vec{\eta}_{ij}) = \frac{\vec{\mathcal{F}}_i^{(k-1)} + \vec{\mathcal{F}}_j^{(k-1)}}{2} \cdot \vec{\eta}_{ij} \tag{20}$$

In the advection case the resulting FCT scheme writes :

$$\Phi_{ij}^{lim} = \Phi_{ij}^{low} + l_{ij} \left(\Phi_{ij}^{high} - \Phi_{ij}^{low} \right) \tag{21}$$

where the l_{ij} are defined following [13, 14, 21]. By the following algorithm : Put

$$W_i^{min} = \min_{\substack{j = i \\ and\ j\ neighbor\ of\ i}} (W_i^n, W_i^{n+1,low})$$

$$W_i^{max} = \max_{\substack{j = i \\ and\ j\ neighbor\ of\ i}} (W_i^n, W_i^{n+1,low})$$

where W_i^n, $W_i^{n+1,low}$ results from (**??**)-(**??**) and then :

$$P_i^+ = - \sum_{j\ neighbor\ of\ i} \min(0, \Phi_{ij}^{low} - \Phi_{ij}^{high})$$

$$P_i^- = + \sum_{j\ neighbor\ of\ i} \max(0, \Phi_{ij}^{low} - \Phi_{ij}^{high})$$

$$Q_i^+ = d_i W_i^{max} - \sum_{j \neq i} \Phi_{ij}^{low}$$

$$Q_i^- = \sum_{j \neq i} \Phi_{ij}^{low} - d_i W_i^{min}$$

$$R_i^+ = \begin{cases} 0 & si\ P_i^+ = 0 \\ 1 & si\ Q_i^+ \geq P_i^+\ et\ P_i^+ \neq 0 \\ \frac{Q_i^+}{P_i^+} & si\ Q_i^+ \leq P_i^+\ et\ P_i^+ \neq 0 \end{cases} \tag{22}$$

$$R_i^- = \begin{cases} 0 & si\ P_i^- = 0 \\ 1 & si\ Q_i^- \geq P_i^-\ et\ P_i^- \neq 0 \\ \frac{Q_i^-}{P_i^-} & si\ Q_i^- \leq P_i^-\ et\ P_i^- \neq 0 \end{cases} \tag{23}$$

and finally

$$l_{ij} = \min(R_i^+, R_i^-, R_j^+, R_j^-)\ ;$$

by construction we have the

Lemma : *If the first order scheme satisfies the Maximum Principle (resp. positiveness), then so does the FCT scheme.*

Remark 3 : Note that scheme (**??**) should be used with a stability CFL condition that is the most pessimistic of the conditions corresponding to (**??**) and (**??**). In general, an accurate enough multi–step procedure is more stable than the Godunov one step. Further, Runge–Kutta schemes stay very accurate for time steps several times smaller than the maximum admissible.

Remark 4 : It is also possible for CPU cost reduction to use the Godunov step as the first step of the multi–step high order scheme.

Remark 5 : Another option is to use as high order scheme an upwind one as constructed in the sequel.

Remark 6 : For an extension to general hyperbolic systems, see for example [21].

5 MUSCL Variants

The above Godunov scheme (Section 3) is a first–order accurate scheme obtained by adding to the high– order (at least second–order) finite element scheme an internal viscosity in terms of second order derivatives. We describe now a second–order Godunov scheme which is a perturbation of the Finite Element scheme by (essentially) a numerical viscosity in terms of fourth order derivatives, similarly to second order accurate upwind schemes.

Indeed, following van Leer, we can replace in the Approximate Riemann Solver the nodal values W_i and W_j by "better" interpolations :

$$\Phi_{ij}^{high,\ upwind} = \Phi^{ROE}(W_{ij}, W_{ji}, \vec{\eta}_{ij})$$

with

$$W_{ij} = W_i + (\vec{\nabla} W)_{ij}\ .\ \frac{\vec{ij}}{2}$$

where $(\vec{\nabla} W)_{ij}$ is an approximation of ∇W near node i. Several choices are possible (see for the P1 case [Aachen]) ; in order to possibly obtain a fully upwind scheme, we suggest the "upwind element construction" [Atlanta, Reno], in which the gradient $(\vec{\nabla} W)_{ij}$ is computed from node values taken in the first element accross which vector $\vec{ji}$ is pointing as sketched in Figure 3.

Figure 3 : upwind element for segment $\vec{ij}$

At last it is possible to introduce some anti–oscillatory limiter ; we have been employing for a long time the van Albada limiter [VL].

$$\begin{aligned} W_{ij}^{lim} &= W_i + \ ave\ (a,b) \\ a &= \vec{\nabla} W_{ij} \ . \ \frac{\vec{ij}}{2} \\ b &= Wj - Wi \\ ave\ (a,b) &= \frac{(a^2+\epsilon)b+(b^2+\epsilon)a}{a^2+b^2+2\epsilon}\ if\ ab > 0 \\ &= 0\ otherwise \end{aligned}$$

where ϵ is a small positive number.

However this construction is yet rather heuristic in this 2D context ; rigorously non–oscillating schemes are hardly derived ; we refer to [18] for an attempt starting for a multi–dimensional extension of Harten's incremental condition.

Remark 7 : The first–order variant can be used for first–order linear preconditioning [19] or defect correction [20] since it enjoys matrix properties favourable to relaxation.

Remark 8 : The MUSCL formulation can also be applied to combine the first order Godunov scheme to the central–differenced finite–element scheme as sketched (in P1 case) in [7]. In this particular case, we can imagine to keep the consistant mass matrix (with a loss of robustness).

Remark 9 : The above spatial scheme can also be advanced in time by a multi–step Runge–Kutta Scheme.

6 CONCLUDING REMARKS

The presented schemes enjoy many of the interesting properties of their ingredients :

– easy and rational derivation of first and second derivatives, on possibly heterogeneous meshes (triangles combined with quadrilaterals), relaxing the constraint of node by node consistency through a variational point of view.

– positiveness preservation (at least for first–order Godunov and scalar FCT) and, more generally, stabilization terms allowing discontinuity capturing (high Mach), and collocated meshes without spurious pressure nodes.

For the MUSCL construction, or more generally for a TVD construction, a rigorous theory for 2D / 3D monotonicity preservation is really missing. This could also allow progress in the capture of 2D shocks, since they can be potentially thinly captured by a central differencing combined to an adhoc numerical viscosity.

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