Development of Cell-vertex Multidimensional Upwind Solvers for the Compressible Flow Equations

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This paper describes the results of a three year study on multidimensional upwind fluctuation-splitting schemes for the Euler equations. It discusses successively: (1) a multidimensional wave model allowing the decoupling of the system in a number of scalar wave contributions suitable for application of the scalar advection schemes; (2) a multidimensional conservative Roe-linearization for the system of Euler equations in two space dimensions; (3) multidimensional monotonic and high-resolution scalar advection schemes on triangles; (4) optimal multi-stage schemes for the multidimensional scalar advection operators; (5) a multigrid solver for the Euler system on structured quadrilateral meshes, based on the optimal explicit smoothing operators.

1 Introduction

The equations for inviscid non-heat-conducting flow, known as the Euler equations, form a hyperbolic system of conservation laws for mass, momentum and energy, in which information travels along particular directions called characteristics. It is well known, for instance, that in one-dimensional unsteady *subsonic* flows, disturbances travel both upstream and downstream, whereas they travel only downstream in *supersonic* flows. Recognizing the wave-like nature of compressible flows was crucial to the development of the first successful method for computing transonic flows [1]. Since then, the development of numerical methods for solving the multidimensional Euler equations with improved shock-capturing properties has been a very important research topic in CFD. Two general methodologies have competed in the last decades, the first one based on central differencing and artificial dissipation, the second one relying on the concept of upwinding. This second method is favored by the authors for its capability of somehow mimicking the physics of wave propagation phenomena. Indeed, for the one-dimensional case, upwind methods based on the solution of Riemann problems have reached a remarkable level of accuracy, at a reasonable computational cost.

Extension to more than one dimension has been based mostly on directional splitting, thereby misinterpreting the multidimensional physics of the flow. To overcome this difficulty, truly multidimensional upwind methods have been investigated.

A first approach, in the framework of Finite Volume methods, is based on the concept of "rotated" Riemann solvers [2], for which informations are no longer constrained to propagate in grid-normal directions, but in more physical directions (flow, pressure gradient, etc.)

A second more general approach, followed in this work, is based on the concept of "fluctuation-splitting", and finds its natural application on cell-vertex grids: the cell residuals are decomposed in a set of scalar waves, propagating in solution-dependent directions, and each wave contribution is then distributed to the cell vertices using newly-developed high-resolution advection schemes.

During the three-year research, the method has strongly improved in all specific areas relating to the basic methodology: new, more robust wave-models, which allow the residual decomposition, have been devised; a conservative linearization has been developed; new genuinely multidimensional schemes for scalar advection equations have been discovered, which are both accurate and monotonic; finally, optimally smoothing multi-stage schemes combined with efficient multigrid procedures have been developed and implemented for scalar advection equations and generalized to the Euler equations. This paper provides a global description of this research.

2 Governing equations

The 2D Euler equations in integral and divergence forms are given respectively as:

$$\frac{\partial}{\partial t}\iint_{\Omega} \mathbf{U}\, d\Omega + \oint_{\partial\Omega} \mathcal{F}\cdot \vec{ds} = 0, \tag{2.1}$$

where $\mathbf{U}$ is the vector of conserved variables, $\mathcal{F} = \mathbf{F}\vec{1}_x + \mathbf{G}\vec{1}_y$ the flux vector and $\vec{ds}$ an elementary normal along the contour $\partial\Omega$, orientated towards the exterior of the domain Ω.

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{pmatrix} \qquad \mathbf{G} = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v H \end{pmatrix}$$

ρ is the density of the gas, u and v are the x and y components of the velocity vector $\vec{u}$, p is the static pressure, E the specific total energy and $H = E + \frac{p}{\rho}$ the specific total enthalpy. The system is closed by the Equation of State which in the case of a perfect gas may be written:

$$p = (\gamma - 1)\rho\left(E - \frac{1}{2}(u^2 + v^2) \right)$$

γ is the ratio of specific heats, $c = \sqrt{\gamma p/\rho}$ is the speed of sound. Useful expressions for the previous quantities are:

$$\begin{aligned} E &= \frac{p}{\rho(\gamma-1)} + \frac{1}{2}(u^2+v^2) \\ H &= \frac{\gamma}{\gamma-1}\frac{p}{\rho} + \frac{1}{2}(u^2+v^2) \\ c^2 &= (\gamma-1)[H - \frac{1}{2}(u^2+v^2)] \end{aligned}$$

Applying Gauss's theorem to (2.1) and assuming Ω fixed in space, one obtains:

$$\iint_\Omega (\mathbf{U}_t + \nabla\cdot\mathcal{F}\,)\,d\Omega = 0$$

from which the divergence form of the Euler equations is obtained:

$$\mathbf{U}_t + \mathbf{F}_x + \mathbf{G}_y = 0. \tag{2.2}$$

Important properties characterizing the hyperbolic nature of the Euler system can be derived from its quasi-linear form. In conservative variables, one has

$$\mathbf{U}_t + \left(\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\right)\mathbf{U}_x + \left(\frac{\partial \mathbf{G}}{\partial \mathbf{U}}\right)\mathbf{U}_y = 0. \tag{2.3}$$

It is often easier to work with the so-called primitive variables. Defining $\mathbf{V} = (\rho,\ u,\ v,\ p\ )^\tau$ as the vector of primitive variables, and $\mathbf{P} = \frac{\partial \mathbf{U}}{\partial \mathbf{V}}$ as the Jacobian of the transformation, one obtains:

$$\mathbf{V}_t + \mathbf{A}\mathbf{V}_x + \mathbf{B}\mathbf{V}_y = 0, \tag{2.4}$$

where $\mathbf{A} = \mathbf{P}^{-1}\ \frac{\partial \mathbf{F}}{\partial \mathbf{U}}\ \mathbf{P}$ and $\mathbf{B} = \mathbf{P}^{-1}\ \frac{\partial \mathbf{G}}{\partial \mathbf{U}}\ \mathbf{P}$.

The Euler equations are hyperbolic so that the matrix $\mathbf{C}_m = \mathbf{A}\cos\theta + \mathbf{B}\sin\theta$ has real eigenvalues for all values of θ, namely:

$$\lambda_m^{1,2} = \vec{u}\cdot\vec{m} \qquad \lambda_m^{3,4} = \vec{u}\cdot\vec{m} \pm c$$

where $\vec{m} = \cos\theta\vec{1}_x + \sin\theta\vec{1}_y$. The corresponding right (column) and left (row) eigenvectors, representing respectively an entropy wave, a shear wave, a "fast" acoustic wave and a "slow" acoustic wave, are given by:

$$[\mathbf{r}] = \begin{bmatrix} 1 & 0 & \rho/c & \rho/c \\ 0 & -\sin\theta & \cos\theta & -\cos\theta \\ 0 & \cos\theta & \sin\theta & -\sin\theta \\ 0 & 0 & \rho c & \rho c \end{bmatrix}, \qquad [\mathbf{l}] = \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{c^2} \\ 0 & -\sin\theta & \cos\theta & 0 \\ 0 & \frac{\cos\theta}{2} & \frac{\sin\theta}{2} & \frac{1}{2\rho c} \\ 0 & -\frac{\cos\theta}{2} & -\frac{\sin\theta}{2} & \frac{1}{2\rho c} \end{bmatrix}.$$

The right eigenvectors in conservative variables are obtained from the transformation $[\mathbf{R}] = \mathbf{P}[\mathbf{r}]$:

$$[\mathbf{R}] = \begin{bmatrix} 1 & 0 & \rho/c & \rho/c \\ u & -\rho\sin\theta & (\rho u + \rho c\cos\theta)/c & (\rho u - \rho c\cos\theta)/c \\ v & \rho\cos\theta & (\rho v + \rho c\sin\theta)/c & (\rho v - \rho c\sin\theta)/c \\ \dfrac{u^2+v^2}{2} & -\rho(u\sin\theta - v\cos\theta) & (\rho H + \rho c\vec{u}\cdot\vec{m})/c & (\rho H - \rho c\vec{u}\cdot\vec{m})/c \end{bmatrix}.$$

A simple wave solution of (2.4) is a solution of the form $\mathbf{V} = \mathbf{V}(W)$, where $W = W(x, y, t)$ is a scalar. For such a solution, one has:

$$\nabla\mathbf{V} = \frac{d\mathbf{V}}{dW}\nabla W, \qquad \frac{\partial\mathbf{V}}{\partial t} = \frac{d\mathbf{V}}{dW}\frac{\partial W}{\partial t}.$$

These, combined with (2.4), and defining $\vec{m}$ as the unit vector in the direction of ∇W, $\nabla W = \mid \nabla W \mid \ \vec{m}$, provide

$$\left[\frac{\partial W}{\partial t}\mathbf{I} + (\mathbf{A}m_x + \mathbf{B}m_y) \mid \nabla W \mid\right]\frac{d\mathbf{V}}{dW} = 0, \tag{2.5}$$

which admits non-trivial solutions only if $\frac{d\mathbf{V}}{dW}$ is a right eigenvector of $\mathbf{C}_m$, and $-\frac{1}{|\nabla W|}\frac{\partial W}{\partial t}$ the corresponding eigenvalue, namely:

$$\frac{d\mathbf{V}}{dW} = \mathbf{r}, \qquad -\frac{1}{\mid \nabla W \mid}\frac{\partial W}{\partial t} = \lambda_m. \tag{2.6}$$

The last equation can be rewritten as a scalar advection equation:

$$\frac{\partial W}{\partial t} + \vec{\lambda}_m \cdot \nabla W = 0, \tag{2.7}$$

where $\vec{\lambda}_m$, called the *frontal speed*, is defined as $\vec{\lambda}_m = \lambda_m \ \vec{m}$. Equation (2.7) has solutions of the form

$$W(x, y, t) = W(q), \qquad q = xm_x + ym_y - \lambda_m t. \tag{2.8}$$

Equation (2.6) can thus be rewritten as:

$$\nabla\mathbf{V} = \mathbf{r}\nabla W = \alpha\, \mathbf{r} \ \ \vec{m},$$

where $\alpha = \frac{d\mathbf{W}}{dq}$ represents the strength of the wave.

3 Multidimensional upwind schemes

3.1 Wave models

The first step in the construction of multidimensional upwind schemes is the development of a wave model, which generalizes to 2D the eigenvector decomposition used in all upwind methods for the 1D Euler equations. This idea is explained in more detail in [3, 4, 5]. Multidimensional wave models have already been proposed in 1986 following two independent approaches, one by ROE [6] based on simple waves, and one by DECONINCK ET AL. [7] based on characteristic theory. These models have been further refined. For lack of space, only the simple wave approach is considered here.

As shown by ROE [6], a finite number of the above simple wave solutions modeling elementary flow patterns, can be combined to match any variation of the data. For example, in the case of a 6-wave model, one has in primitive variables,

$$\nabla \mathbf{V} = \sum_{k=1}^{6} \alpha_k \mathbf{r}_k \vec{m}_k, \tag{3.1}$$

and in conservative variables,

$$\nabla \mathbf{U} = \sum_{k=1}^{6} \alpha_k \mathbf{R}_k \; \vec{m}_k. \tag{3.2}$$

Thus, the flux divergence can be decomposed as:

$$\nabla \cdot \mathcal{F} = \sum_{k=1}^{6} \alpha_k \lambda_m^k \mathbf{R}_k. \tag{3.3}$$

Notice that, contrary to the 1D case, this decomposition is not unique so that different wave models can be chosen. The first two proposed by ROE [6] (models A and B) consisted of a set of four acoustic waves, propagating normal to each other, an entropy wave propagating in the direction of the entropy gradient, and a measure of vorticity (model A) or shear, perpendicular to the velocity (model B), to take care of rotational effects. During the first year of this project, no satisfactory results were obtained using either model A or B. Therefore, a variant (model C) was constructed [8], with the shear wave propagating in the direction of the pressure gradient. In this model, the 6 waves chosen are: 4 acoustic waves, with strengths $\alpha_1, \alpha_2, \alpha_3, \alpha_4$, propagating in directions $\theta, \theta + \frac{\pi}{2}, \theta + \pi, \theta + \frac{3\pi}{2}$; 1 entropy wave, with strength $\alpha_5 = \beta$, propagating in the direction ϕ; 1 shear wave, with strength $\alpha_6 = \sigma$, propagating in the direction of ∇p. The expressions for the wave strengths and angles are:

$$\begin{aligned}
\beta &= \sqrt{\left(\rho_x - \frac{p_x}{c^2}\right)^2 + \left(\rho_y - \frac{p_y}{c^2}\right)^2}, \\
\phi &= \arctan_{[0,2\pi]} \frac{\rho_y - \frac{p_y}{c^2}}{\rho_x - \frac{p_x}{c^2}}, \\
\sigma &= v_x - u_y, \\
\psi &= \arctan_{[0,2\pi]} \frac{p_y}{p_x}, \\
\theta &= \frac{1}{2} \arctan_{[0,2\pi]} \frac{u_y + v_x - \sigma \cos 2\psi}{u_x - v_y + \sigma \sin 2\psi},
\end{aligned}$$

$$\alpha_{1,3} = \frac{1}{2}\left[\frac{u_x+v_y+R}{2} \pm \frac{p_x\cos\theta + p_y\sin\theta}{\rho c}\right],$$
$$\alpha_{2,4} = \frac{1}{2}\left[\frac{u_x+v_y-R}{2} \mp \frac{p_x\sin\theta - p_y\cos\theta}{\rho c}\right],$$

where R is defined as

$$R = \frac{u_y+v_x-\sigma\cos 2\psi}{\sin 2\theta} = \frac{u_x-v_y+\sigma\sin 2\psi}{\cos 2\theta}.$$

This model, as will be shown, allows good capturing of discontinuities, although convergence down to machine zero is not achieved in most cases. To remedy the problem, it was proposed to send the shear wave in the direction of the velocity vector $\vec{u}$. This model, called here model E, was used in the first-order multigrid computations [9], with convergence to machine zero in all cases. The reason is that the direction of the shear wave does not depend on gradients, which are much more sensitive to noise than the velocity direction and are ill-defined in regions of uniform flows.

In the meantime, a new model (model D) was developed by Roe [10], for which the shear wave is sent at 45^o to the acoustic wave. Consequently, for an isolated shock wave, the acoustic waves are found to propagate in the directions normal and parallel to the discontinuity and for an isolated shear layer, the shear wave propagates in the direction normal to the discontinuity. Such a model appears to be the most consistent with the multidimensional wave propagation phenomena associated with the Euler equations and will be studied further in the future. Some preliminary results are included in this paper.

3.2 Conservative linearization, fluctuations and speeds

3.2.1 Conservative linearization

The multidimensional generalization of Roe's original 1D Flux Difference Splitter [11] is an essential feature of the overall method, insofar as it allows the use of quasi-linear forms while guaranteeing conservation. It was discovered independently by Roe and members of the present team [3, 12, 13]. The main ideas are summarized here.

A fundamental assumption is that of piecewise linear data. In 2D, linear elements are triangles. We thus consider triangular (unstructured or not) meshes, with unknowns stored at the vertices, just as in linear Finite Elements. The parameter vector $\mathbf{Z} = (\sqrt{\rho},\ \sqrt{\rho}u,\ \sqrt{\rho}v,\ \sqrt{\rho}H\ )^\tau$ is assumed to vary linearly over each triangle. Since $\frac{\partial \mathbf{U}}{\partial \mathbf{Z}}$, $\frac{\partial \mathbf{F}}{\partial \mathbf{Z}}$,and $\frac{\partial \mathbf{G}}{\partial \mathbf{Z}}$ are linear functions of $\mathbf{Z}$, their integrals over a triangle are easily obtained in terms of the average state $\bar{\mathbf{Z}}$ over the cell, $\bar{\mathbf{Z}} = \frac{1}{3}[\mathbf{Z}_1 + \mathbf{Z}_2 + \mathbf{Z}_3]$, where indices $1, 2, 3$ denote the vertices of that cell. One can define average gradients such as:

$$\widehat{\nabla \mathbf{U}} = \frac{1}{S_T}\iint_T \nabla \mathbf{U}\, d\Omega, \qquad \widehat{\mathbf{F}}_x = \frac{1}{S_T}\iint_T \mathbf{F}_x\, d\Omega, \qquad \widehat{\mathbf{G}}_y = \frac{1}{S_T}\iint_T \mathbf{G}_y\, d\Omega.$$

As a consequence of the previous assumption,

$$\begin{aligned}
\widehat{\mathbf{F}}_x &= \frac{1}{S_T}\iint_T \frac{\partial \mathbf{F}}{\partial \mathbf{Z}}\mathbf{Z}_x\, d\Omega = \left(\frac{\partial \mathbf{F}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\mathbf{Z}_x, \qquad & \widehat{\mathbf{G}}_y = \left(\frac{\partial \mathbf{G}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\mathbf{Z}_x,\\
\widehat{\mathbf{U}}_x &= \left(\frac{\partial \mathbf{U}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\mathbf{Z}_x, & \widehat{\mathbf{U}}_y = \left(\frac{\partial \mathbf{U}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\mathbf{Z}_y.
\end{aligned}$$

From the equations above, one obtains:

$$\mathbf{Z}_x = \left(\frac{\partial \mathbf{U}}{\partial \mathbf{Z}}\right)^{-1}_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_x, \qquad \mathbf{Z}_y = \left(\frac{\partial \mathbf{U}}{\partial \mathbf{Z}}\right)^{-1}_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_y.$$

Thus,

$$\begin{aligned}
\oint_{\partial T}\mathcal{F}\cdot\vec{ds} &= \iint_T(\mathbf{F}_x+\mathbf{G}_y)\,d\Omega = S_T\left[\widehat{\mathbf{F}}_x+\widehat{\mathbf{G}}_y\right]\\
&= S_T\left[\left(\frac{\partial \mathbf{F}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\left(\frac{\partial \mathbf{Z}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_x+\left(\frac{\partial \mathbf{G}}{\partial \mathbf{Z}}\right)_{\bar{\mathbf{Z}}}\left(\frac{\partial \mathbf{Z}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_y\right]\\
&= S_T\left[\left(\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_x+\left(\frac{\partial \mathbf{G}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_y\right].
\end{aligned}$$

The linearization is conservative, namely:

$$(1) \qquad \sum_T S_T[\widehat{\mathbf{F}}_x+\widehat{\mathbf{G}}_y] = \sum_T\oint_{\partial T}\mathcal{F}\cdot\vec{ds} = \oint_{\partial\Omega_{outer}}\mathcal{F}\cdot\vec{ds}$$

$$(2) \qquad \widehat{\mathbf{F}}_x+\widehat{\mathbf{G}}_y = \left[\left(\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_x+\left(\frac{\partial \mathbf{G}}{\partial \mathbf{U}}\right)_{\bar{\mathbf{Z}}}\widehat{\mathbf{U}}_y\right].$$

The first statement characterizes the "telescopic property" of the residuals: the only terms left after summation involve the outer boundaries of the domain. The second statement shows that for each triangle the quasilinear form of the flux divergence is an exact expression for the flux divergence.

For linearly varying $\mathbf{Z}$ the gradients of the primitive variables, needed to compute the wave strengths and angles, see (3.1), can be computed exactly as:

$$\widehat{\nabla\mathbf{V}} = \begin{pmatrix} 2\sqrt{\bar\rho}\nabla(\sqrt{\rho})\\ \frac{1}{\sqrt{\bar\rho}}[\nabla(\sqrt{\rho}u)-\bar u\nabla(\sqrt{\rho})]\\ \frac{1}{\sqrt{\bar\rho}}[\nabla(\sqrt{\rho}v)-\bar v\nabla(\sqrt{\rho})]\\ \frac{\gamma-1}{\gamma}\sqrt{\bar\rho}[\bar H\nabla(\sqrt{\rho})-\bar u\nabla(\sqrt{\rho}u)-\bar v\nabla(\sqrt{\rho}v)+\nabla(\sqrt{\rho}H)]\end{pmatrix}.$$

The wave decomposition of the gradient of $\mathbf{U}$ at the average state $\bar{\mathbf{Z}}$,

$$\widehat{\nabla\mathbf{U}} = \sum_{k=1}^{6}\bar\alpha_k\bar{\mathbf{R}}_k\,\vec{m}_k,$$

combined with the conservative property stated above, gives an exact expression for the flux divergence:

$$\widehat{\mathbf{F}}_x + \widehat{\mathbf{G}}_y = \sum_{k=1}^{6} \bar{\alpha}_k \bar{\lambda}_m^k \bar{\mathbf{R}}_k.$$

Thus, the expression for the residual over a triangle T is:

$$\Phi_T = -\oint_{\partial T} \mathcal{F} \cdot \vec{ds} = -S_T \sum_{k=1}^{6} \bar{\alpha}_k \bar{\lambda}_m^k \bar{\mathbf{R}}_k = \sum_{k=1}^{6} \Phi_T^k. \tag{3.4}$$

3.2.2 Fluctuations and speeds

The residual in cell T has been split into 6 wave contributions. Each wave is associated to an advection equation in a pseudo-characteristic variable $\bar{W}^k$, given by eq.(2.7) :

$$\frac{\partial \bar{W}^k}{\partial t} + \vec{\bar{\lambda}}_m^k \cdot \nabla \bar{W}^k = 0,$$

where $\bar{W}^k(x,y,t) = \bar{\alpha}_k(\vec{x} \cdot \vec{m}_k - \bar{\lambda}_m^k t)$ and $\nabla \bar{W}^k = \bar{\alpha}_k \vec{m}_k$. For each wave, one can define the scalar fluctuation and the residual in conservative variables as:

$$\phi_T^k = -\iint_T \vec{\lambda}_m^k \cdot \nabla \bar{W}^k \, d\Omega, \tag{3.5}$$

$$\Phi_T^k = \phi_T^k \, \bar{\mathbf{R}}_k. \tag{3.6}$$

For the case of supersonic flow, the frontal speed $\vec{\bar{\lambda}}_m^k$ may project the fluctuation outside the domain of dependence, see Figure 3.1. This unphysical "behaviour" can be cured by using the ray speeds $\vec{\lambda}^k$, given by:

$$\vec{\lambda}_e = \vec{u}, \quad \vec{\lambda}_s = \vec{u}, \quad \vec{\lambda}_a = \vec{u} + c\,\vec{m}. \tag{3.7}$$

FIGURE 3.1. Acoustic ray and frontal speeds (soundspeed c and Mach angle μ)

This is allowed thanks to the important property that the fluctuation is invariant for any choice of $\vec{\lambda}^k$ such that $\vec{\bar{\lambda}}_m^k = (\vec{\bar{\lambda}}^k \cdot \vec{m}_k)\vec{m}_k$:

$$\phi_T^k = -S_T \vec{\bar{\lambda}}_m^k \cdot \nabla \bar{W}^k = -S_T \vec{\bar{\lambda}}^k \cdot \nabla \bar{W}^k = -S_T \bar{\lambda}_m^k \mid \nabla \bar{W}^k \mid = -S_T \bar{\lambda}_m^k \bar{\alpha}_k . \quad (3.8)$$

Therefore, for each wave, the fluctuation will be convected according to the advection equation:

$$\frac{\partial \bar{W}^k}{\partial t} + \vec{\bar{\lambda}}^k \cdot \nabla \bar{W}^k = 0. \tag{3.9}$$

Finally, the expression for the scalar fluctuation ϕ_T^k given by (3.8) can be rewritten, using Gauss' theorem, as:

$$\phi_T^k = -\iint_T \vec{\lambda}^k \cdot \nabla \bar{W}^k \, d\Omega = \sum_{i=1}^{3} k_i \bar{W}_i^k \tag{3.10}$$

where

$$k_i = \frac{1}{2} \vec{\bar{\lambda}}^k \cdot \vec{n}_i \tag{3.11}$$

and $\vec{n}_i$ are the inward normals of the triangle T, scaled with the lengths of the sides, as shown in Figure 3.2.

FIGURE 3.2. Generic triangle

3.3 Scalar advection schemes

For each wave, the residual $\Phi_T^k = \phi_T^k \bar{\mathbf{R}}_k$ is split between the three nodes of the triangle in an upwind manner: only the downstream node(s) receive(s) a contribution. Note that from now onward, the average sign will be omitted for convenience.

The accuracy and quality of the solution depends on: (1) the advection scheme; (2) the quality of the grid, in particular for structured grids, the choice of the diagonal subdividing each quadrilateral cell into two triangles; and (3) the wave-model. Considerable research has been devoted to the study of multi-dimensional scalar advection schemes [14, 15, 16]. A number of schemes has been devised and three important properties have been identified: positivity, linearity-preservation and continuity. A scheme is said to be positive if it preserves monotonicity, and linearity-preserving if it preserves piecewise linear solutions. For linear schemes, i.e., of the form $W_i^{n+1} = \sum c_k W_k^n$, where c_k are independent of the data, this last property was shown in [15] to be equivalent to second-order accuracy on orthogonal Cartesian grids, based on a method developed in [17]. Finally, a desirable property of a scheme is continuity of the distribution, for continuously varying advection speed and gradients. An important theorem, generalizing Godunov's theorem, states that a linear scheme cannot be both positive (P) and linearity preserving (LP). This is the main reason for studying non-linear schemes. In this paper, we limit ourselves to a discussion of three continuous schemes:

1. the N scheme: optimal linear P scheme
2. the Low Diffusion A (LDA) scheme: linear LP scheme
3. the PSI scheme: non-linear P and LP scheme

Other non-linear schemes have been proposed by Roe in [18]. All schemes can be written in the following form: for a given triangle T and wave k, the residual at node i receives a contribution

$$\mathbf{Res}_i \to \mathbf{Res}_i + \beta_{i,k}^T \Phi_T^k = \mathbf{Res}_i + \gamma_{i,k}^T \mathbf{R}_k,$$

where $\beta_{i,k}^T$ are weighting coefficients such that $\sum_i \beta_{i,k}^T = 1$ for conservation ($\sum_i$ represents the summation over the three nodes of the triangle) and the $\gamma_{i,k}^T$ sum up to the scalar fluctuation for the cell, ϕ_T^k.

3.3.1 N scheme

This scheme, proposed by Roe in [19], is the optimal linear positive scheme. In the case of the one-inflow triangle shown in figure 3.3, the upwind strategy suggests sending all of the fluctuation to the unique downstream node N_3:

$$\mathbf{Res}_3 \to \mathbf{Res}_3 + \mathbf{\Phi}_T^k. \tag{3.12}$$

For the two-inflow triangle shown in Figure 3.4, with downstream nodes N_1 and N_2, the fluctuation is split according to the decomposition of the advection speed $\vec{\lambda}$ along the sides of the triangles:

$$\vec{\lambda} = \vec{\lambda}_1 + \vec{\lambda}_2.$$

For each component $\vec{\lambda}_i$, the triangle is a one-inflow triangle and (3.12) can be used. The contributions to each node are:

$$\mathbf{Res}_1 \to \mathbf{Res}_1 - k_1(W_1 - W_3)\mathbf{R}_k, \tag{3.13}$$

$$\mathbf{Res}_2 \to \mathbf{Res}_2 - k_2(W_2 - W_3)\mathbf{R}_k, \tag{3.14}$$

where $(W_1 - W_3)$, for example, can be computed as $\nabla W \cdot \vec{N_3 N_1}$. This scheme can be cast into the single formula [20],

$$\gamma_{i,k}^T = \frac{\max(0,k_i)}{\sum_{j=1}^3 \max(0,k_j)} \sum_{j=1}^{3} \left[\min(0,k_j)(W_i - W_j)\right]. \tag{3.15}$$

FIGURE 3.3. One-inflow case

FIGURE 3.4. Two-inflow case: N

3.3.2 LDA scheme

This scheme is linear and LP (hence non-positive). For the two-inflow triangle, the advection vector $\vec{\lambda}$ divides the triangle into two sub-triangles. The splitting is then based on the ratios of the areas of these triangles to the area of the original one, see Figure 3.5. The coefficients $\beta_{1,2}^T$ are thus given by:

$$\beta_1^T = \frac{Area_{342}}{Area_{123}} = -\frac{k_1}{k_3}, \tag{3.16}$$

$$\beta_2^T = \frac{Area_{314}}{Area_{123}} = -\frac{k_2}{k_3}, \tag{3.17}$$

which sum up to one since $\sum_i k_i = 0$. Again, this scheme can be cast into a concise formula:

$$\gamma_{i,k}^T = \frac{\max(0,k_i)}{\sum_{j=1}^3 \max(0,k_j)} \phi_T^k. \tag{3.18}$$

3.3.3 PSI scheme

The Positive Streamwise Invariant (PSI) scheme is a non-linear P and LP scheme, which fulfills solution invariance along streamlines. Again, for one-inflow triangles, the entire residual is sent to the downstream node. For two-inflow triangles, the strategy is the following:

1. if $(\vec{N_3N_1} \cdot \vec{m})(\vec{N_3N_2} \cdot \vec{m}) > 0$, the line of constant W through the upstream node is outside $[N_1, N_2]$, then apply the N scheme;

2. else, the line of constant W goes through $[N_1, N_2]$ as shown in Figure 3.6 and positivity constraints lead to the following one-target distributions:

- if $\alpha_k(\overrightarrow{N_2N_1} \cdot \vec{m})\phi_T^k = (\overrightarrow{N_2N_1} \cdot \nabla W)\phi_T^k > 0$, send everything to N_1,
- else, send everything to N_2.

A general formula for the downstream nodes ($i = 1, 2$) is given by:

$$\gamma_{i,k}^T = \frac{\max(0, k_i)\ \min\left[0, (W_i - W_3)\phi_T^k\right]}{\sum_{j=1}^3 \left[\max(0, k_j) \min\left(0, (W_j - W_3)\phi_T^k\right)\right]}\ \phi_T^k.$$

FIGURE 3.5. Two-inflow case: LDA

FIGURE 3.6. Two-inflow case: PSI

3.4 General scheme and time-marching

The explicit forward Euler time-stepping scheme is described here as the simplest iterative technique to obtain steady state. The optimal multi-stage time-integration scheme used in the multigrid computations will be described in Section 4.

The residual at each node is first computed by looping over all triangles. For each triangle, the wave residuals are distributed according to the chosen scalar advection scheme

$$\mathbf{Res}_i = \sum_T \sum_k \beta_{i,k}^T \Phi_T^k, \tag{3.19}$$

where $\sum_T$ refers to the summation over all triangles having i as common vertex. The updating of the state vector $\mathbf{U}$ at node i is then given as:

$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{S_i}\mathbf{Res}_i. \tag{3.20}$$

In this equation, S_i is the area of the median dual cell around node i (equal to one third of the area of all triangles having i as a vertex) and Δt the time-step chosen with the following restriction, based on the worst case over all waves [15]:

$$\Delta t \leq \Delta t_{\max} = \frac{S_i}{\sum_T \max(0, k_i^T)}. \tag{3.21}$$

4 Optimal explicit smoothing for multigrid acceleration on quadrilateral grids

4.1 Motivation

The availability of vector and parallel processors and the use of local refinement as a basic tool for obtaining high resolution results to complex flow problems have increased the interest in using explicit schemes as smoothers in multigrid methods for the Euler equations, as an alternative to classical relaxation schemes. Indeed, multigrid methods work also for hyperbolic problems for two reasons: low frequency errors are convected out of the domain faster, thanks to the increased numerical propagation speed resulting from the coarse grid correction, and high frequency errors are eliminated by damping, thanks to the dissipation always present in both central and upwind discretizations. Therefore, it appears logical and worthwhile to extend the idea of optimizing the high frequency damping properties of a multi-stage scheme [21] to the present framework of genuinely multidimensional upwind schemes, as proposed in [22, 23, 24] and brought to maturity in this paper.

4.2 Scalar advection

4.2.1 Space-time discretization

Consider the 2D linear advection equation

$$\frac{\partial u}{\partial t} = -\vec{\lambda} \cdot \nabla u = -a\frac{\partial u}{\partial x} - b\frac{\partial u}{\partial y} = \mathrm{Res}(u), \quad \frac{a}{\Delta x} \geq \frac{b}{\Delta y} \geq 0,\ a \neq 0, \quad (4.1)$$

defined in a bounded domain with prescribed initial conditions and Dirichlet boundary conditions. The physical domain is divided (grid h) into $m \times n$ rectangular cells $\Delta S_{i,j}$ with constant mesh-sizes Δx and Δy and with the unknowns located at each cell-vertex. Eq.(4.1) is firstly semi-discretized in space, the associated semi-discrete equation being formally written as:

$$\left(\frac{\partial u}{\partial t}\right)_{i,j} = \left(L^h(u)\right)_{i,j}, \quad (4.2)$$

where L^h is the spatial differencing operator defined on the grid h and applied at point (i,j). As an example, consider the standard first-order-accurate upwind (SU) scheme, in its finite difference formulation:

$$\Delta t\,\frac{\partial u}{\partial t} = -\frac{a\Delta t}{\Delta x}\,[u(x,y,t)-u(x-\Delta x,y,t)]-\frac{b\Delta t}{\Delta y}\,[u(x,y,t)-u(x,y-\Delta y,t)]. \quad (4.3)$$

The time differencing operator in (4.2) is then analyzed by (Fourier) transforming (4.3), as follows:

$$\frac{du}{dt} = \frac{\nu z}{\Delta t}\,u, \quad z \in C, \quad \nu = \max(\nu_x, \nu_y) = \max\left(\frac{a\Delta t}{\Delta x}, \frac{b\Delta t}{\Delta y}\right). \quad (4.4)$$

In (4.4), $z = z(\beta_x, \beta_y, \vartheta)$ is proportional to the Fourier transform of L^h. β_x and β_y are the spatial wave numbers in the two coordinate directions and ϑ is the convection angle, defined as $\vartheta = \arctan(R) = \arctan(\nu_y/\nu_x)$. For the SU scheme, one has

$$z = \left(e^{-i\beta_x} - 1\right) + R\left(e^{-i\beta_y} - 1\right) \ . \tag{4.5}$$

In the case of a general coordinate system (ξ, η), (4.1) is re-written as:

$$\frac{\partial u}{\partial t} = -(\vec{\lambda} \cdot \nabla\xi)\frac{\partial u}{\partial \xi} - (\vec{\lambda} \cdot \nabla\eta)\frac{\partial u}{\partial \eta} \tag{4.6}$$

and the definitions of ν and R are generalized as:

$$\nu = \max(\nu_\xi, \nu_\eta), \quad R = \min\left(\frac{\nu_\xi}{\nu_\eta}, \frac{\nu_\eta}{\nu_\xi}\right), \quad \nu_\xi = \vec{\lambda} \cdot \nabla\xi\Delta t, \ \nu_\eta = \vec{\lambda} \cdot \nabla\eta\Delta t. \tag{4.7}$$

The interest of the authors is focused in developing an efficient smoother for the N scheme described previously in Section 3.3.1. When using a structured grid, each quadrilateral cell has to be subdivided into two cells. Due to the degree of freedom in the choice of the diagonal, different stencils can be obtained. It can be shown that, for a linear equation on a uniform Cartesian grid, the N scheme recovers the positive linear scheme with minimum cross-diffusion [17] if the diagonal most aligned with the advection speed vector is used; alternatively, the classical dimensionally-split SU scheme is obtained. Therefore, an optimal diagonal choice can be performed in each cell, which allows in particular to improve the resolution of discontinuities.

FIGURE 4.1. a) Equally-oriented grid; b) Isotropic grid

For the two configurations in Figure 4.1, the function $z(\beta_x, \beta_y, R)$ takes a different form, depending on the shape of the grid and the direction of the advection speed vector $\vec{\lambda}$, see [9] for details.
Finally, the time derivative of the ordinary differential equation (4.4) is discretized by the multi-stage explicit Runge-Kutta (RK) scheme

$$u^{(0)} = u^{\ell}, \tag{4.8}$$
$$u^{(k)} = u^{(0)} + c_k \nu z \ u^{(k-1)} \ , \ k = 1, ..., n, \tag{4.9}$$
$$u^{\ell+1} = u^{(n)}, \tag{4.10}$$

whose properties will be analyzed in the following.

4.2.2 Smoothing analysis

The amplification factor for the RK-scheme of (4.8-4.10) is the following polynomial function of degree n

$$P_n(z) = 1 + c_n \nu z(1 + c_{n-1} \nu z(...(1 + c_1 \nu z))). \tag{4.11}$$

The n parameters $c_k,\ k = 1, ..., n-1$ and ν have to be chosen so as to maximize the smoothing properties of the scheme, rather than satisfying its time accuracy, since the interest is limited to steady state. Here, an equivalent and more convenient expression is used for $P_n(z)$; if n is even, the RK-scheme can be analyzed as a sequence of m predictor-corrector schemes, namely:

$$P_n(z) = \prod_{k=1}^{m} (1 + \nu_k z + \alpha_k \nu_k^2 z^2), \qquad n = 2m. \tag{4.12}$$

Otherwise, if n is odd, one forward Euler step has to be added:

$$P_n(z) = (1 + \nu_{m+1} z)\ P_{2m}(z), \qquad n = 2m + 1. \tag{4.13}$$

As in the formulation (4.11), n coefficients — namely m parameters α_k and $(m+p)$ parameters ν_k $(p = n-2m)$ — have to be fixed. Consider a 1D equation, for simplicity. The goal is to control the magnitude of the amplification factor $\rho = \|P_n(z)\|$ in the high frequency range $[\pi/2, \pi]$, namely, to minimize its maximum value σ (smoothing factor). The complete mathematical formulation of the minmax problem is the following:

$$\sigma_{opt} = \min_{\vec{\alpha}, \vec{\nu}} \left[\max_{\beta \in [\pi/2, \pi]} \|P_n(z(\beta), \vec{\alpha}, \vec{\nu})\| \right], \tag{4.14}$$

where $\vec{\alpha} = (\alpha_1, ..., \alpha_m)$ and $\vec{\nu} = (\nu_1, ..., \nu_{m+p})$. In [21], $P_n(z)$ was forced to have $m+p$ zeroes $\beta_{0,k}$ in the high frequency range and the problem was reduced to

$$\sigma_{opt} = \min_{\vec{\beta}_0} \left[\max_{\beta \in [\pi/2, \pi]} \|P_n(z(\beta), \vec{\beta}_0)\| \right], \tag{4.15}$$

$\vec{\alpha}$ and $\vec{\nu}$ being expressed as functions of the vector $\vec{\beta}_0 = (\beta_{0,1}, ..., \beta_{0,m+p})$. The simplified problem (4.15) is equivalent to (4.14) only in the case of first-order upwind differencing. In all other cases, the solution of (4.15) does not produce the optimal coefficients, although a satisfactory smoothing is achieved anyway, see [22]. More importantly, the technique proposed in [21], using (4.15) as goal function, cannot be extended to the 2D analysis, where a zero of ρ is a two-component vector $(\beta_{0,x}, \beta_{0,y})$. For these reasons, a different and more general approach is proposed using the original parameters α_1, ..., α_m, ν_1, ..., ν_{m+p}, rather than β_1, ..., β_m.

4.2.3 Optimization technique

Consider a first-order upwind $2m$-stage scheme in one dimension: for such a discrete operator, the square of the magnitude of the amplification factor ρ^2 has no more than $n+1=2m+1$ local extrema in $[0,\pi]$. Two of them are located respectively in $\beta=0$ and $\beta=\pi$, for symmetry. Since $\rho^2(\beta)$ is continuous together with its derivatives, a minimum (maximum) is located between two successive maxima (minima). Therefore the number of *possible* maxima in $[0,\pi]$ is $\bar{N}=\sup\ \mathrm{int}[(n+1)/2]=m+1$. When considering only the high frequency range $[\pi/2,\pi]$, $\bar{N}$ is again m+1, since the boundary value $\rho(\beta=\pi/2)$ has to be included, while the value $\rho(\beta=0)$ has to be excluded (similarly, for an odd number of stages ($n=2m+1$), $\bar{N}=\sup\ \mathrm{int}[(n+1)/2]=m+1$). Incidentally, in all numerical experiments, it has been found that the smoothing factor is minimized when the number of maxima N_{max} in the high frequency range is equal to $\bar{N}$.

A simple gradient method is not well suited for solving (4.14), since the function $\sigma(\vec{\alpha},\vec{\nu})$ is not differentiable when two or more maxima are equal: in fact, small perturbations of $\vec{\alpha}$ and $\vec{\nu}$ around this position, move the location of σ from one maximum to another. The present strategy aims at eliminating such discontinuities before applying the gradient method. First consider the case of a 2-stage scheme with $N_{max}=\bar{N}=m+1=2$; under the equal excursion principle, the two maxima M_0 and M_1 must be equal, namely:

$$M_0(\alpha,\nu)=M_1(\alpha,\nu)\ . \tag{4.16}$$

In [21], the optimal β_0 was calculated from the nonlinear Equation (4.16), thus solving the minmax problem (4.15) directly. Here, (4.16) is used as a condition for expressing α as a function of ν. The fulfillment of (4.16) makes the function $\sigma(\alpha(\nu),\nu)=\sigma(\nu)$ always differentiable with respect to ν: in fact, the derivative $d\sigma(\alpha(\nu),\nu)/d\nu$ is defined in the singular sub-domain $\alpha=\alpha(\nu)$, determined by (4.16), in which σ coincides with either of the maxima. The smoothing factor is then minimized by imposing the following condition, that completes the set of two equations in the two unknowns α and ν,

$$\frac{d\sigma(\alpha(\nu),\nu)}{d\nu}=0\ . \tag{4.17}$$

It is noteworthy that using (4.17) is more appropriate than forcing a zero of ρ [21], which does not guarantee the optimum. Eqs.(4.16) and (4.17) can be solved analytically for first-order upwind differencing. In a more general case, a numerical approach is required: 1) a solution (α^0,ν^0) with $N_{\max}=\bar{N}=2$ is guessed; 2) α is evaluated from (4.16) using the Newton-Raphson technique, keeping ν constant; in such a way, a new solution $(\alpha^1,\nu^1=\nu^0)$, satisfying the condition $M_0=M_1=\sigma$, is obtained; 3) the derivative $d\ \sigma/d\nu$ is evaluated numerically, with $\alpha=\alpha(\nu)$ calculated from (4.16) and the value of ν is then increased or decreased, always satisfying (4.16), depending on the sign of $d\sigma/d\nu$, until the minimum is reached.

Consider now the more general case of n stages and $1 < N_{\max} \leq \bar{N} = m+1$: the vector $\vec{\alpha}$ can be decomposed as $\vec{\alpha} = \vec{\alpha}_{grad} + \vec{\alpha}_{\max}$, where $\vec{\alpha}_{grad} = (\alpha_1, ..., \alpha_{m-N_{\max}+1}, 0, ..., 0)$ and $\vec{\alpha}_{\max} = (0, ..., 0, \alpha_{m-N_{\max}+2}, ..., \alpha_m)$. For $N_{\max} = 1$, it results in $\vec{\alpha}_{\max} = \vec{0}$ and $\vec{\alpha}_{grad} = \vec{\alpha}$, while for $N_{\max} = \bar{N}$ one has $\vec{\alpha}_{\max} = \vec{\alpha}$ and $\vec{\alpha}_{grad} = \vec{0}$. The $N_{\max}$ maxima are again imposed to be equal:

$$M_k(\vec{\alpha}, \vec{\nu}) = M_{k-1}(\vec{\alpha}, \vec{\nu}), \qquad k = 1, ..., N_{\max} - 1. \tag{4.18}$$

This allows to express the $(N_{\max} - 1)$ nonzero components of $\vec{\alpha}_{\max}$ as functions of the remaining parameters. Finally, the first partial derivatives of the differentiable function $\sigma(\vec{\alpha}_{\max}(\vec{\alpha}_{grad}, \vec{\nu}) + \vec{\alpha}_{grad}, \vec{\nu}) = \sigma(\vec{\alpha}_{grad}, \vec{\nu})$ with respect to the components of $\vec{\nu}$ and to the non-null components of $\vec{\alpha}_{grad}$ are set to zero:

$$\frac{\partial \sigma(\vec{\alpha}_{grad}, \vec{\nu})}{\partial \nu_k} = 0, \qquad k = 1, ..., m+p, \tag{4.19}$$

$$\frac{\partial \sigma(\vec{\alpha}_{grad}, \vec{\nu})}{\partial \alpha_{grad,k}} = 0, \qquad k = 1, ..., m - N_{\max} + 1 \ . \tag{4.20}$$

The numerical procedure described above is easily extended to the general case of n stages and $N_{\max} \leq \bar{N}$: in the step 1), a solution $(\vec{\alpha}^0, \vec{\nu}^0)$ is guessed; step 2) consists in calculating $\vec{\alpha}_{\max}$ from (4.18) by means of a Newton iteration: the differences

$$R_k = M_k - M_{k-1}, \qquad k = 1, ..., N_{\max} - 1, \tag{4.21}$$

are defined as the components of the residual vector $\vec{R}$. Suppose that the actual solution is $(\vec{\alpha}^i, \vec{\nu}^i)$; in the next gradient step, the updated value $\vec{\alpha}^{i+1}_{\max} = \vec{\alpha}^i_{\max} + \Delta\vec{\alpha}_{\max}$ has to satisfy (4.18), that is, $\vec{R} = \vec{0}$. Starting from $\vec{\alpha}^{i,0}_{\max} = \vec{\alpha}^i_{\max}$, the solution is updated as $\vec{\alpha}^{i,j}_{\max} = \vec{\alpha}^{i,j-1}_{\max} + \Delta\vec{\alpha}^j_{\max}$, the correction $\Delta\vec{\alpha}^j_{\max}$ being calculated from the linearized expression of $\vec{R} = \vec{0}$:

$$\frac{\partial \vec{R}^{j-1}}{\partial \vec{\alpha}_{\max}} \ \Delta\vec{\alpha}^j_{\max} = -\vec{R}^{j-1}. \tag{4.22}$$

The maxima $M_k, \ k = 0, 1, ..., N_{\max} - 1$, as well as the Jacobian matrix $\partial\vec{R}^{j-1}/\partial\vec{\alpha}_{\max}$, are evaluated numerically. by a updated. The value $\vec{\alpha}^{i,j}_{\max}$ is updated until $\vec{R} = \vec{0}$. Step 3) consists again in a classical gradient method: the partial derivatives in (4.19) and (4.20) are continuous and are evaluated numerically as well. $N_{\max}$ is eventually updated at each gradient step.
The entire optimization procedure can be extended to the 2D case, keeping in mind some very important recommendations: firstly, it appears from (4.5) that the Fourier transform of L^h depends on the CFL ratio R; therefore, the smoothing properties of the scheme, as well as the corresponding optimal coefficients and time step, will depend on R as well. In two dimensions, the domain of definition of $P_n(z)$ is the square

$$\{\beta_x \in [0,\pi],\ \beta_y \in [0,\pi]\},$$

$P_n(z)$ being point symmetric with respect to the x and y axes, while the high frequency region is defined as

$$\{\pi/2 \le \underline{\beta} \le \pi;\ \underline{\beta} = \max(\beta_x, \beta_y)\}. \tag{4.23}$$

The smoothing factor must be defined in the domain determined by (4.23). However, for $R \to 0$, namely, when the advection direction is aligned with one of the coordinate lines (in this case the x axis), one has $z\,(\beta_x = 0, \beta_y) \to 0$, for consistency, and therefore $P_n \to 1$. No smoothing can be provided for the waves $\beta_x = 0$; moreover, the attempt of minimizing the smoothing factor results in a reduced stability of the scheme for all waves, since the entire amplification factor field is raised up and even set to 1 in the extreme case $R = 0$. For a genuinely 2D scheme, a similar situation occurs also for the waves $\beta_x = \beta_y$ when the advection involves only the diagonal grid points ($R = 1$). Such a problem was already seen in [23], when considering a scalar advection equation, and overcome by using an exact linearized advection speed and limiting the domain of definition of σ. However, the first procedure cannot be extended to the case of the Euler equations, see [24]. In conclusion, the domain of definition of σ must exclude the waves that produce a unitary amplification factor, for consistency, namely:

$$\left\{\pi/2 \le \underline{\beta} \le \pi;\ \underline{\beta} = \max(\beta_x, \beta_y)\,;\ \beta_x > 0,\ \beta_y > 0\right\}. \tag{4.24}$$

In the case of schemes capable of convecting signals along the diagonal grid points exactly, the frequency $(\beta_x = \pi, \beta_y = \pi)$ must be excluded as well. Referring to the optimization procedure described above, the boundary maximum is a local extreme on the line

$$\{0 < \beta_x \le \pi/2, \beta_y = \pi/2\} \cup \{\beta_x = \pi/2, 0 < \beta_y < \pi/2\}, \tag{4.25}$$

whereas the interior maxima have to be searched in the *restricted* high frequency domain defined by (4.24), see Figure 4.2. The coefficients used in the Euler calculations are provided in [9, 24].

5 Results

Solutions of a scalar advection equation are first computed for different schemes and choices of the diagonals. Solutions of the Euler equations are then presented with emphasis on discontinuity-capturing and multigrid.

5.1 Results for scalar convection

The scalar advection equation

$$u_t + \vec{\lambda} \cdot \nabla u = 0$$

is considered, with constant speed $\vec{\lambda} = \vec{1}_x + \vec{1}_y$. The fluctuation over a cell, (3.5), becomes:

FIGURE 4.2. High and low frequency Fourier domain

$$\phi_T = \iint_T u_t \, dx \, dy = -S_T \vec{\lambda} \cdot \nabla u.$$

The linear and non-linear schemes are tested on three different grids, *parallel* (diagonals aligned with $\vec{\lambda}$), *perpendicular* (diagonals normal to $\vec{\lambda}$) and *isotropic* (alternating diagonals), on the domain $0 \leq x \leq 1, 0 \leq y \leq 1$. Dirichlet boundary conditions are imposed: $u = 3.0$ on $y = 0$, $u = 5.0$ on $x = 0$. The state at point (0,0) is set at the average state $u = 4.0$.

The N scheme captures the steady discontinuity exactly (in two rows of cells) only for the *parallel* grid: in that case, all triangles are one-inflow and so the entire residual (which is zero) is sent to the downstream node, thereby preserving the exact steady state. For the *perpendicular* and *isotropic* grids, the solution spreads: for the two-inflow triangles, the zero fluctuation is split into two non-zero components and the exact solution is destroyed.
The LDA scheme preserves linear solutions; therefore, in the case of the *parallel* and *isotropic* grids, for which the exact solution can be mapped linearly onto the mesh, the solution is preserved. For the *perpendicular* grid, the solution spreads, and a non-monotone profile is obtained.
The PSI scheme, like the LDA scheme, is linearity preserving. Therefore, it preserves the exact steady solution on the *parallel* and *isotropic* grids. For the *perpendicular* grid, the solution spreads though less than for the N scheme, and contrary to the LDA scheme, a monotonic solution is obtained.
All schemes converge to machine zero with no difficulties.

5.2 Results for the Euler equations using simple time-stepping

In this section, the multidimensional schemes for the Euler equations are first tested on non-smooth steady flows, which, in the case of inviscid compressible flows, are either shock waves or slip lines. Particular attention is focused on the ability of the fluctuation splitting schemes to resolve or "capture" the discontinuities. A detailed study of a nonlinear scalar conservation law [25] is of great help in understanding the mechanism of wave splitting. The different scalar advection schemes are tested and compared to one another on several test-cases, involving normal and oblique shocks, shear layers, a jet interaction and the transonic flow over an airfoil. The convergence properties of the schemes are also assessed.

5.2.1 Normal and oblique shock

A normal shock is considered. States upstream and downstream of the shocks are related by the Rankine-Hugoniot jump relations for normal shocks, which in this case give for $M_1 = 2.0$, $\rho_1 = 1.0$ and $p_1 = 1/\gamma$, $M_2 \approx 0.57$,$\rho_2 \approx 2.66$, and $p_2 = 4.5/\gamma$.
The discontinuity is taken aligned with the mesh, and periodic boundary conditions are imposed. In this case, all triangles are one-inflow, for which the one-target update formula is both positive and linearity preserving. Just as in the scalar case, the profiles (not shown) contain three cells or two intermediate states.
The next test-case is an oblique shock at 45^o to the freestream flow, with a deflection angle of about 14^o, and upstream and downstream Mach numbers $M_1 = 1.98$ and $M_2 = 1.45$. Densities are respectively $\rho_1 = 3.11$ and $\rho_2 = 5.29$. The N scheme and the PSI scheme are tested here on an isotropic grid, with model C. The Mach number contours are plotted for each scheme. For the N scheme, Figure 5.1 shows that the solution is spread over the grid. Convergence stalls after a drop of about three orders of magnitude in the density residual. In the case of the PSI scheme, the discontinuity is captured exactly, with one intermediate state, as shown in Figure 5.2. Convergence is satisfactory, with a drop of four orders of magnitude in the residual.

5.2.2 Shear aligned with the grid

A shear with a density jump is computed on an isotropic mesh. Conditions are $M_1 \approx 2.6$ and $M_2 \approx 4.8$, $\rho_1 = 1.0$ and $\rho_2 = 2.0$ and equal pressure across. The PSI scheme was used with model C and D. Clearly, model C, which uses the direction of the pressure gradient, ill-defined across a shear layer, is not robust for such a case. Better results are obtained with model D, both in terms of accuracy and convergence. Figure 5.3 shows the Mach number contours obtained with model C: the discontinuity is found to spread a little. On the contrary, it is kept perfectly with model D, as seen in Figure 5.4.

5.2.3 Jet interaction

In this section, the fluctuation splitting schemes are compared to a standard finite volume scheme, Roe's Flux Difference Splitting (FDS) scheme [11]. The comparison is made on a test-case cited by Glaz and Wardlaw [26]: a pure Riemann problem consisting in the interaction of two supersonic parallel jets, for which an exact solution can be computed. The upper stream, denoted (1), at conditions $M_1 = 4.0$, $\rho_1 = 0.50$ and $p_1 = 0.25$; the lower stream, denoted (2), at conditions $M_2 = 2.4$, $\rho_2 = 1.0$ and $p_2 = 1.0$. The interaction of the two jets produces a shock wave propagating in the low pressure region and an expansion fan propagating in the high pressure region, with a contact discontinuity in between.

Solutions were computed with the N and PSI schemes using model C, as well as with a first and second-order FDS scheme. For the fluctuation splitting schemes, the cell-vertex isotropic grid consists of 41×41 nodes, on the domain $[0,1] \times [0,1]$, corresponding to the 40×40 cell-centered mesh used in the FDS calculations.

Density contours for the four different computations are plotted in Figures 5.5, 5.6, 5.7 and 5.8. It appears that the N scheme is better than the first-order FDS scheme, but less accurate than the second-order one, whereas the PSI scheme is comparable to the second-order FDS scheme.

Convergence stagnates after a drop of about 1.5 orders of magnitude in the residual. As anticipated in Section 3.1, model C does not converge to machine accuracy whenever there are regions of zero pressure gradient.

5.2.4 Transonic NACA 0012 airfoil

A transonic flow ($M_\infty = 0.85$, angle of attack 1^o) is computed around a NACA 0012 airfoil, on a structured O-type mesh with 128×32 nodes. The grid with fixed diagonals is shown in Figure 5.9. The far-field is at 20 chords and the far-field boundary conditions are not corrected with the required circulation. The numerical solution is computed using model D and the nonlinear PSI scheme. The Mach number contours are given in Figure 5.10, showing well-defined shocks on both pressure and suction sides of the airfoil. Convergence for the PSI scheme with model D stagnates after a residual drop of 3 orders of magnitude.

5.3 Multigrid results for the Euler equations

The smoother described in Section 4 is designed to work effectively in conjunction with a multigrid method. Here, the well-known FMG FAS V-cycle of Brandt [27] is employed, with one pre- and one post-application of the aforementioned three-stage Runge–Kutta smoother, at all levels. The choice of the grid transfer operators is briefly outlined: the defect $d^h_{i,j} = -\mathbf{Res}_{i,j}$ is computed at each grid point (i,j) of the mesh h and collected onto the coarser grid $H{=}2h$ using classical full-weighting. The coarse grid correction is then transferred back to the finer grid by standard bilinear interpolation. This solver, proven effective for scalar advection equations [24], is now applied to Roe's six wave decomposition model E using the first-order N scheme spatial discretization described previously.

As shown before, the choice of the diagonal affects the accuracy of the N scheme, also when used in conjunction with the multi-dimensional Euler solver. However, since the propagation direction is not unique in this case, the selected diagonal cannot be optimal for all of the waves. Two strategies have been an-

alyzed, namely: 1) since the wave with largest $\bar{\alpha}^k$ within a cell is the one that locally dominates the flow behaviour, its propagation direction defines the optimal diagonal, as described before [28]; 2) in presence of shocks, the diagonal more aligned with the discontinuity is selected [9].
Characteristic boundary conditions are imposed at subsonic inlet and outlet: total enthalpy, entropy and flow angle are specified at inflow boundaries, while the pressure is specified at outlet. At the wall, the equations are integrated also in a row of auxiliary cells outside of the physical domain; the mirror-image flow conditions are calculated by imposing impermeability and isentropic simple radial equilibrium [9, 29]. The multigrid Euler solver has been tested versus three subsonic, transonic [9] and supersonic [24] flow problems.

5.3.1 Subsonic and transonic GAMM channel

For the first two cases, the flow through the GAMM channel is calculated for two different values of the inlet Mach number, using a 129×65 uniform non-orthogonal isotropic grid. The iso-Mach lines for the subsonic case ($M_i = 0.6$) are shown in Figure 5.11. The solution is rather symmetric: the small shift at the lower wall shows that a small amount of numerical dissipation is introduced in the re-compression region. Convergence to machine zero is obtained, as well as in the other two cases, see Figure 5.12, where the single- and the multigrid convergence histories are presented: the logarithm of the L^1-norm of the residual of the mass conservation equation is plotted versus the work, one *work unit* being again defined as *one single-stage residual* calculation on the *finest grid*. The FMG FAS V-cycle strategy discussed before has been employed, the time step being unique for all waves and based on the fastest one. Even without any characteristic time stepping, a considerable gain in work is achieved. The reduction in the convergence rate, seen at $R \approx -2.5$, is due to the well-known multigrid alignment phenomenon: error modes of low frequency along the streamlines and high frequency in the transversal direction are created near the lower wall and can be neither smoothed by the time integration, nor convected out from the domain by the coarser grids. Semi-coarsening should reduce such a problem.
Similar considerations apply to the solution of the transonic flow case ($M_i = 0.83$) shown in Figure 5.13. A further decrease in the MG convergence rate is experienced in this case (see Figure 5.14), since no extra-relaxations are applied in the shock region.

5.3.2 Shock reflection on a flat wall

Finally, the well known shock-reflection problem has been considered, the oblique shock impinging upon a flat plate at a 29 degree angle, see Figure 5.15, where the solution obtained using a 193×65 uniform isotropic grid and the N scheme is presented. The shock resolution is typical of a good first-order-accurate genuinely multidimensional method and can be easily improved by using the diagonal choice strategy described above, see Figure 5.17. Obviously, use of a non-linear scheme like the PSI leads to better shock resolution as seen previously in Figures 5.1 and 5.2. Single grid and multigrid convergence histories are shown in Figures 5.16 and 5.18: the single grid solution is rather fast, thanks to the hyperbolic nature of the spatial problem; nevertheless, a considerable reduction in work is achieved when using multigrid, in both cases. The comparison between Figures 5.15 and 5.18 shows that no significant increase in computational time [9] is required by the adaptive solver, in spite of its improved shock resolution.

CONCLUSIONS

A major step forward in the development of multidimensional cell-vertex upwind schemes for hyperbolic conservation laws has been made during this project. Wave models based on Roe's simple wave decomposition have been further developed and tested, providing a two-dimensional decomposition of the flux divergence into scalar contributions. Contrary to grid-aligned decompositions, the models allow the recognition of shocks and shears for multidimensional flow without reference to the grid.

Linear as well as non-linear scalar advection schemes have been further developed and successfully applied to each of the scalar wave contributions of the Euler residual. The nonlinear PSI scheme is monotone and preserves linear solutions. It allows similar discontinuity-capturing properties as standard high-resolution upwind schemes on much more compact stencils, involving only direct neighbours. On structured grids, the choice of the diagonal for splitting the quadrilaterals represents an additional degree of freedom to improve the accuracy and discontinuity capturing. Such an automatic diagonal optimization procedure has been devised and implemented with success.

A significant step towards the overall success of the methodology has been made by devising a general conservative linearization of the Euler equations over triangles. This allows the use of quasilinear expressions without any loss of conservation.

The above developments have led to the first working Euler solver based on fluctuation-splitting and simple wave modelling.

An explicit multi-stage smoother has been designed for general two-dimensional advection operators. Its effectiveness has been firstly demonstrated in a multigrid code for scalar equations, using several genuinely multi-dimensional upwind schemes. Then, the explicit multigrid strategy has been extended to the wave-decomposition of 2D Euler equations. A significant efficiency improvement has been achieved in all cases analyzed.

The solver has been tested for a wide range of applications including shocks, shears, airfoils and channels at subsonic, transonic and supersonic speeds. This demonstrates the validity of the new concepts introduced which can be seen as a major breakthrough in compressible Computational Fluid Dynamics.

Further work is still needed for improving the robustness of wave models when used in combination with high-order schemes, and in the areas of linearization, boundary conditions and multigrid. Finally, extension to Navier-Stokes and 3 space dimensions has to be considered.

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FIGURE 5.1. Oblique shock: N

FIGURE 5.2. Oblique shock: PSI

FIGURE 5.3. Shear: PSI/model C

FIGURE 5.4. Shear: PSI/model D

FIGURE 5.5. Jet: N/model C

FIGURE 5.6. Jet: Roe $1^{st}\mathcal{O}$

FIGURE 5.7. Jet :PSI/model C

FIGURE 5.8. Jet: Roe $2^{nd}\mathcal{O}$

FIGURE 5.9. NACA airfoil: structured mesh (128×32 O-mesh)

FIGURE 5.10. NACA airfoil: Mach contours - PSI/model D

FIGURE 5.11. Subsonic channel: Mach contours - N/model E

FIGURE 5.12. Subsonic channel: convergence histories

FIGURE 5.13. Transonic channel: Mach contours - N/model E

FIGURE 5.14. Transonic channel: convergence histories

FIGURE 5.15. Shock reflection: Mach contours - N/model E (isotropic grid)

FIGURE 5.16. Shock reflection: convergence histories (isotropic grid)

FIGURE 5.17. Shock reflection: Mach contours - N/model E (grid with adapted diagonals)

FIGURE 5.18. Shock reflection: convergence histories (grid with adapted diagonals)