DEPARTMENT OF AEROSPACE ENGINEERING

Faculty Name	:	**Dr.A.Arun Negemiya, ASP/ Aero**	Academic Year	:	**2024-2025 (Even)**
Year & Branch	:	**III AEROSPACE**	Semester	:	**VI**
Course	:	**19ASB304 - Computational Fluid Dynamics for Aerospace Application**			

UNIT IV – FINITE VOLUME TECHNIQUES

Cell-centered Formulation

Cell Centered Formulation

For a cell as shown in Fig. 4.5, the values of the dependent variables are stored in the center of the cell. These values do not necessarily have to be seen as nodal values, but can also be seen as mean values over the cell. Therefore, in the cell-centered method, for visualization purposes, often, after completion of the calculations, values are attributed to the vertices of the grid by taking a weighted mean of the values in adjacent cells. Further, the interpretation as mean values allows higher-order formulation, as we discuss in Sect. 4.6. First, we discuss the typical second-order accurate formulations.

Using the control volume of Fig. 4.5, a semi-discretization of (4.1) is obtained By

$$\Omega_{i,j}\frac{\partial U}{\partial t} + \int_{abcd} \vec{F}.\vec{n}\,dS = 0$$

where $\Omega_{i,j}$ denotes the volume (area) of the control volume. $\vec{F}$ is the flux vector: $\vec{F} = f\,\vec{1}_x + g\,\vec{1}_y$, dS is a surface element and $\vec{n}$ is the outward normal. By taking the positive sense as indicated in the figure, we have

$$\vec{n}\,dS = dy\,\vec{1}_x - dx\,\vec{1}_y$$

Inserting (4.3) into (4.2) gives

$$\Omega_{i,j}\frac{\partial U}{\partial t} + \int_{abcd} (f\,dy - g\,dx) = 0$$

Further, f and g have to be defined on the boundary of the volume. A mean value between

adjacent nodes looks to be the simplest choice, for example:

$$f_{ab} = \tfrac{1}{2}(f_{i,j} + f_{i,j-1}), \qquad g_{ab} = \tfrac{1}{2}(g_{i,j} + g_{i,j-1})$$

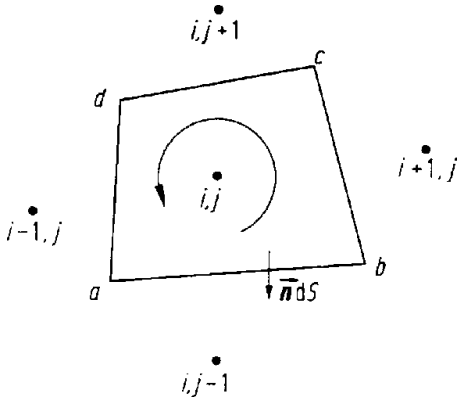

Fig. 4.5 Cell-centred formulation

Since the flux functions are non-linear functions of the dependent variables, an alternative for (4.5) is

$$f_{ab} = f[\tfrac{1}{2}(U_{i,j} + U_{i,j-1})], \qquad g_{ab} = g[\tfrac{1}{2}(U_{i,j} + U_{i,j-1})]$$

With (4.6) it means that the dependent variables are first averaged and that afterward flux vectors are calculated. This is not a popular choice, since it implies about twice as many flux evaluations as (4.5). Indeed, when in a structured quadrilateral grid, there are nx subdivisions in a longitudinal direction and ny subdivisions in a transversal direction, then there are nxny cells, but nx(ny + 1) + ny(nx + 1) cell faces. This does not imply that the work involved in (4.6) is twice as much as the work involved in (4.5). A lot of computational effort can be gained by remarking that a momentum flux is a mass flux multiplied by an average velocity, etc. Nevertheless, the definition (4.5) is the cheapest. Therefore, (4.5) is the only central flux definition used in the following (one-sided flux definitions are also possible, as discussed later). With the definition of the discrete fluxes f and g, the semi-discretization (4.4) is completed. It is now to be integrated in time.

Lax Wendroff Time Stepping

Since Lax-Wendroff time-stepping is a very classic explicit time integration method in the finite difference method, explained in previous chapters, we begin by discussing how this time-stepping can be applied to a finite volume formulation. We first recall the principles of a Lax-Wendroff method with the use of the one-dimensional scalar model equation.

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

A Taylor series expansion to the second order gives

$$u^{n+1} \approx u^n + \Delta t\left(\frac{\partial u}{\partial t}\right)^n + \frac{\Delta t^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n$$

and

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = -\frac{\partial}{\partial t}\left(\frac{\partial f}{\partial x}\right) = -\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial t}\right)$$

or

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial x}\left(a\frac{\partial f}{\partial x}\right)$$

with

$$a = \frac{\partial f}{\partial u}$$

Combination of (4.8) and (4.9) gives

$$u^{n+1} \approx u^n + \Delta t\left(-\frac{\partial f^n}{\partial x}\right) + \frac{\Delta t^2}{2}\frac{\partial}{\partial x}\left(a\frac{\partial f^n}{\partial x}\right)$$

The two-dimensional analog of (4.10) on the Euler equations (4.1) is

$$U^{n+1} \approx U^n + \Delta t\left(-\frac{\partial f^n}{\partial x} - \frac{\partial g^n}{\partial y}\right) + \frac{\Delta t^2}{2}\left\{\frac{\partial}{\partial x}\left[A^n\left(\frac{\partial f^n}{\partial x} + \frac{\partial g^n}{\partial y}\right)\right] + \frac{\partial}{\partial y}\left[B^n\left(\frac{\partial f^n}{\partial x} + \frac{\partial g^n}{\partial y}\right)\right]\right\}$$

Where A and B are the Jacobian matrices of the flux vectors:

$$A = \frac{\partial f}{\partial U} \quad , \qquad B = \frac{\partial g}{\partial U}$$

In the finite-difference method, a discretization of (4.10) or (4.5) is called a one-step Lax-Wendroff method. As explained in previous chapters, a possible procedure is to expand the second-order derivatives in space in (4.10) or (4.5) and to replace these derivatives with central difference approximations. In principle, a finite volume formulation on (4.10) or (4.5) is possible since these equations take the form of a flux balance. The fluxes contain however derivatives.

Since the definition

of derivatives is not simple in the finite volume method, one-step methods are never used. The most popular two-step formulations, such as the Richtmyer variant and the MacCormack variant, can however be used without problems in the FVM.

Further, in the one-step method, the primitive flux balances are lost while these are visible in the two-step formulations. Since the MacCormack variant was explained in previous chapters, we illustrate here how this variant can be formulated in finite volume form.

In the MacCormack variant of the Lax-Wendroff method, (4.8) is written as

$$u^{n+1} = \tfrac{1}{2}u^n + \tfrac{1}{2}\Delta t\left(\frac{\partial u}{\partial t}\right)^n + \tfrac{1}{2}u^n + \tfrac{1}{2}\Delta t\left[\frac{\partial}{\partial t}\left(u + \Delta t\frac{\partial u}{\partial t}\right)\right]^n$$

With (predictor)

$$\overline{u^{n+1}} = u^n + \Delta t\left(\frac{\partial u}{\partial t}\right)^n$$

(4.12) can be written as (corrector)

$$u^{n+1} = \tfrac{1}{2}\left[u^n + \overline{u^{n+1}} + \Delta t\frac{\partial}{\partial t}\overline{u^{n+1}}\right]$$

The discretization by MacCormack of (4.13) and (4.14) is

$$\overline{u_i^{n+1}} = u_i^n - \Delta t\left(\frac{f_{i+1}^n - f_i^n}{\Delta x}\right)$$

$$u_i^{n+1} = \tfrac{1}{2}\left[u_i^n + \overline{u_i^{n+1}} - \Delta t\left(\frac{\overline{f_i^{n+1}} - \overline{f_{i-1}^{n+1}}}{\Delta x}\right)\right]$$

Equations (4.15) and (4.16) form the forward-backward variant. The forward and backward discretizations can be interchanged. In the terminology of ordinary differential equations, the MacCormack method is a predictor-corrector method.

The implementation of the MacCormack variant of the Lax-Wendroff method is rather straightforward. In the forward-backward formulation, in the predictor step in Fig. 4.5, the fluxes at the sides ab, bc, cd, and da are evaluated with function values in the nodes (i,j), (i+1, j), (i, j+1) and (i,j), respectively. In the corrector step, this is (i, j−1), (i,j), (i,j), and (i−1, j).

At inflow and outflow boundaries, the FVM can be used as the FDM. This means that, in general, extrapolation formulas are used to define values in nodes outside the domain. For instance, for a subsonic inflow, it is common practice to extrapolate the Mach number from the flow field and to impose stagnation properties and flow direction. At a subsonic outflow, the reverse can be done, i.e. extrapolation of stagnation properties and flow direction and fixing of a Mach number. Very often, pressure is imposed at the outflow.

At solid boundaries, the convective flux can be set to zero. This means that in the flux through a cell surface on a solid boundary, only the pressure comes in:

$$f\,dy - g\,dx = p\begin{bmatrix} 0 \\ dy \\ -dx \\ 0 \end{bmatrix}$$

The pressure at the boundary can be taken to be the pressure in the cell. Sometimes, as in the

FDM, an extrapolation of pressure is used. It is however not always easy to define extrapolation formulas on distorted or unstructured grids.

Four geometrical variants in the choice of the biasing of the fluxes are possible. Figure 4.6 shows schematically the possibilities for the predictor step. In

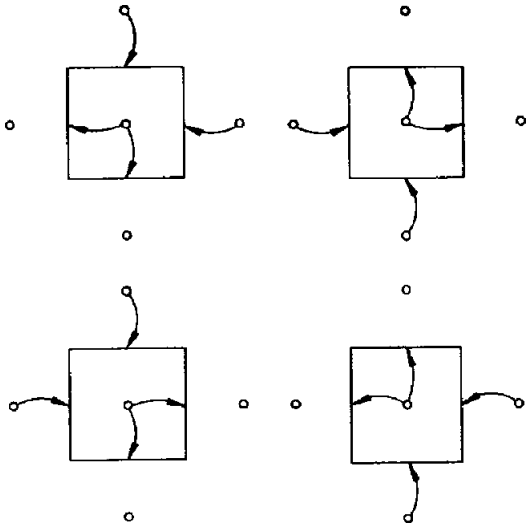

Fig. 4.6 Possible variants of the biasing for flux functions in the predictor step of a MacCormack method

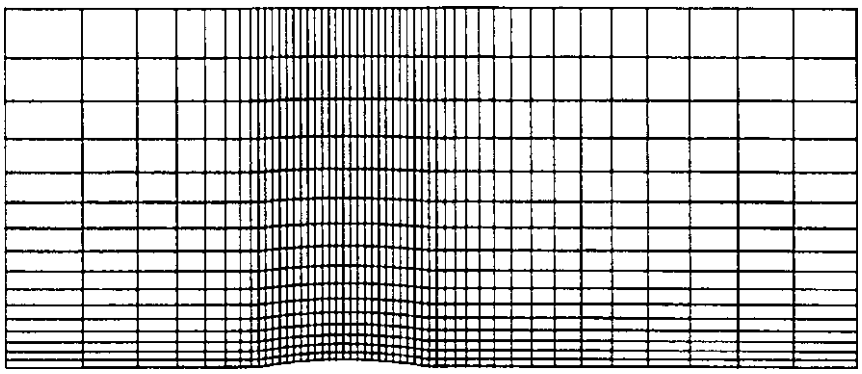

Fig. 4.7 GAMM-channel test problem the corrector step, the biasing is inverted. In practice, the four possibilities are used alternatively.

We illustrate now the cell-centered MacCormack scheme on the well-known GAMM-channel test problem for transonic flows. This problem is shown in Fig. 4.7, discretized with a 49×17 grid. The result shown in Fig. 4.8 is however obtained on a once-refined grid, i.e. a 97×33 grid. The channel of Fig. 4.7 is almost straight except for a small circular perturbation on the lower boundary with height 4.2% of the chord. The result of Fig. 4.8 is obtained with the MacCormack method described above. Pressure is imposed at the outlet, corresponding to an isentropic

Mach number of 0.84. As in the finite-difference method, to obtain this result, some artificial

viscosity is needed to stabilize the solution in the shock region (see discussion in previous chapters). This is done here in a rather primitive way by adding to each step a smoothing of form.

$$\mu\left[U^n_{i+1,j} + U^n_{i-1,j} + U^n_{i,j+1} + U^n_{i,j-1} - 4U^n_{i,j}\right],$$

Where μ is a very small coefficient. For the result in Fig. 4.8: μ = 0.001. This is enough to stabilize the shock. Of course, by increasing μ, the observed wiggles can be eliminated, but this increases the smearing of the shock. Therefore it is preferred to keep some of the wiggles in the solution.

The CFL restriction for the time step in the MacCormack scheme is given by (with c the velocity of sound):

$$\Delta t \le \frac{1}{\frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + c\sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}}}$$

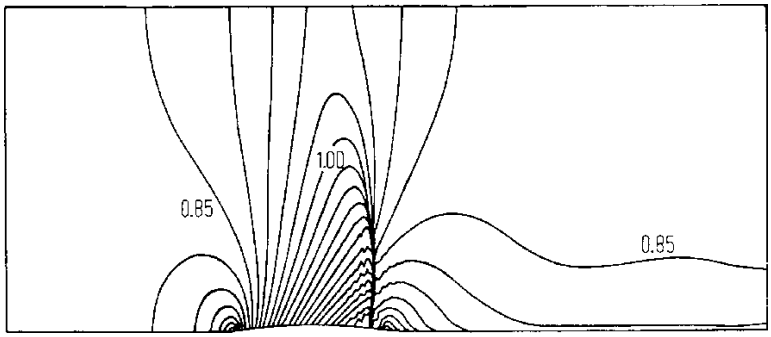

Fig. 4.8 IsoMachlines obtained by cell-centered MacCormack scheme where

$$\Delta x = \frac{x_{i+1,j} - x_{i-1,j}}{2} \quad , \qquad \Delta y = \frac{y_{i,j+1} - y_{i,j-1}}{2}$$

Runge Kutta Time Stepping - Multi-Stage Time Stepping

Runge-Kutta time stepping schemes for ordinary differential equations are unstable when applied to the semi-discretization (4.4) with the central flux (4.5):

$$\begin{aligned}\Omega_{i,j}\frac{\partial U}{\partial t} &+ \tfrac{1}{2}(\Delta y_{ab}\, f_{i,j-1} - \Delta x_{ab}\, g_{i,j-1}) \\ &+ \tfrac{1}{2}(\Delta y_{bc}\, f_{i+1,j} - \Delta x_{bc}\, g_{i+1,j}) \\ &+ \tfrac{1}{2}(\Delta y_{cd}\, f_{i,j+1} - \Delta x_{cd}\, g_{i,j+1}) \\ &+ \tfrac{1}{2}(\Delta y_{da}\, f_{i-1,j} - \Delta x_{da}\, g_{i-1,j}) = 0\end{aligned}$$

There is no contribution of the central node in the flux balance in (4.17) since the flux balance for a constant flux on a closed surface is zero. As a consequence, (4.17) is an exact analog of a

central type finite difference discretization.

The instability of Runge-Kutta time stepping can be seen by considering a Fourier analysis on a central space discretization of the model equation (4.7) for the case of constant $a = \partial f/\partial u$:

$$\frac{\partial u_i}{\partial t} = -a\frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Inserting

$$u = Z\, e^{j\omega x}$$

where ω is the wave-number and j now stands for $\sqrt{-1}$, gives

$$Z' = -Z\, a\frac{e^{j\theta} - e^{-j\theta}}{2\Delta x} = -Z\, ja\frac{\sin\theta}{\Delta x}$$

where $\theta = \omega\Delta x$.

Equation (4.19) has the form

$$Z' = \lambda Z$$

With

$$\lambda = -j\, a\frac{\sin\theta}{\Delta x}$$

Figure 4.9 shows the stability domain for $\lambda\Delta t$ for the Runge-Kutta second, third, and fourth-order, time-integration methods.

Since λ according to (4.20) is on the imaginary axis, the second-order Runge- Kutta method is unstable. Higher-order Runge-Kutta methods are marginally stable.

Higher-order Runge-Kutta methods can be stabilized by introducing a small amount of artificial viscosity. For example, equation (4.18) can be modified to

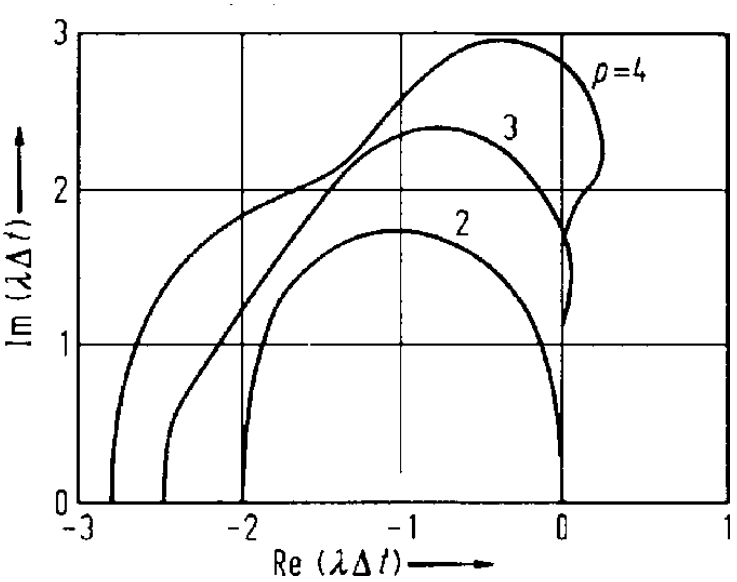

Fig. 4.9 Stability regions in the complex plane for classic explicit Runge-Kutta methods

$$\frac{\partial u}{\partial t} = -a\frac{u_{i+1} - u_{i-1}}{2\Delta x} + \varepsilon\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

The value of λ according to the previous analysis now becomes

$$\lambda = -j\,a\frac{\sin\theta}{\Delta x} - \frac{2\varepsilon}{\Delta x^2}(1 - \cos\theta)$$

Since there is now a small negative real part in λ, higher order Runge-Kutta time stepping now becomes stable, according to Fig. 4.9, when subject to a CFL condition that restricts the time step. Note that a modification of equation (4.18) by adding a fourth-order derivative term instead of a second-order derivative term leads to a similar stabilization effect.

The fourth-order method, with simplifications, is mostly used since it gives the best ratio of allowable time step to computational work per time step. A simplified fourth-order scheme can be written as

$$U_{i,j}^{0} = U_{i,j}^{n}$$

$$U_{i,j}^{1} = U_{i,j}^{0} - \alpha_1 \frac{\Delta t}{\Omega_{i,j}} R^0$$

$$U_{i,j}^{2} = U_{i,j}^{0} - \alpha_2 \frac{\Delta t}{\Omega_{i,j}} R^1$$

$$U_{i,j}^{3} = U_{i,j}^{0} - \alpha_3 \frac{\Delta t}{\Omega_{i,j}} R^2$$

$$U_{i,j}^{4} = U_{i,j}^{0} - \alpha_4 \frac{\Delta t}{\Omega_{i,j}} R^3$$

$$U_{i,j}^{n+1} = U_{i,j}^{4}$$

with $\alpha_1 = {}^1/_4$, $\alpha_2 = {}^1/_3$, $\alpha_3 = {}^1/_2$, $\alpha_4 = 1$
and where the residual R is given by

$$R = \int (f\, dy - g\, dx)$$

And where the superscript denotes the (intermediate) time level.

Obviously (4.21) is not a classic fourth-order Runge-Kutta scheme. In a Runge-Kutta scheme, the fourth step is

$$U_{i,j}^{4} = U_{i,j}^{0} - \alpha_4 \frac{\Delta t}{\Omega_{i,j}} \left(\frac{R^0 + 2R^1 + 2R^2 + R^3}{6} \right)$$

with the choice of coefficients

$$\alpha_1 = {}^1/_2, \quad \alpha_2 = {}^1/_2, \quad \alpha_3 = 1, \quad \alpha_a = 1$$

The accuracy of the fourth-order Runge-Kutta scheme is fourth order in time. This is unnecessarily high since the space accuracy of the discretization is only second order. The simplification (4.21) has second-order accuracy in time for a non-linear equation, which is sufficient. The simplified multi-stage time-stepping (4.21) requires less storage than a classic Runge-Kutta time-stepping. Originally, Jameson used the classic Runge-Kutta method. The low storage modification, later introduced by Jameson, is nowadays universally used.

The scheme (4.21) can be constructed by considering a Taylor expansion up to the fourth order.

$$U^{n+1} \approx U^{n} + \Delta t \frac{\partial U}{\partial t} + {}^1/_2 \Delta t^2 \frac{\partial^2 U}{\partial t^2} + {}^1/_6 \Delta t^2 \frac{\partial^3 U}{\partial t^3} + {}^1/_{24} \Delta t^4 \frac{\partial^4 U}{\partial t^4}$$

The following grouping defines (4.21):

The stability domain of the multi-stage time stepping is the same as that of the fourth-order

$$U^{n+1} \approx U^n + \Delta t \frac{\partial}{\partial t}\left[U^n + {}^1\!/_2 \Delta t \frac{\partial}{\partial t}\left\{U^n + {}^1\!/_3 \Delta t \frac{\partial}{\partial t}\left(U^n + {}^1\!/_4 \Delta t \frac{\partial U}{\partial t}\right)\right\}\right]$$

Runge-Kutta scheme shown in Fig. 4.9.

The artificial viscosity introduced by Jameson is a blend of a second-order and a fourth-order term. It is used in all steps of (4.21).

To keep the calculation conservative, the added dissipative term is, for a structured quadrilateral grid:

$$d_{i+1/2,j} - d_{i-1/2,j} + d_{i,j+1/2} - d_{i,j-1/2}$$

where

$$d_{i+1/2,j} = \varepsilon^{(2)}_{i+1/2,j}(U_{i+1,j} - U_{i,j}) - \varepsilon^{(4)}_{i+1/2,j}(U_{i+2,j} - 3U_{i+1,j} + 3U_{i,j} - U_{i-1,j})$$

With similar definitions of the other terms in (4.22).

The coefficients of the second-order term ε(2) and the fourth-order term ε(4) are chosen in a self-adaptive way.

As a detector of the smoothness of the flow field, for the definition of the coefficients in (4.23), Jameson uses

$$\nu^i_{i,j} = \frac{|p_{i+1,j} - 2p_{i,j} + p_{i-1,j}|}{p_{i+1,j} + 2p_{i,j} + p_{i-1,j}}$$

and then defines

$$\varepsilon^{(2)}_{i+1/2,j} = \kappa^{(2)} \max(\nu^i_{i+1,j}, \nu^i_{i,j})$$
$$\varepsilon^{(4)}_{i+1/2,j} = \max(0, \kappa^{(4)} - \varepsilon^{(2)}_{i+1/2,j})$$

$$\text{with } \kappa^{(2)} = {}^1\!/_4,\ \kappa^{(4)} = {}^1\!/_{256}.$$

By this definition, the second-order term is only significant in shock regions. In smooth regions of the flow, the second-order term has a very small coefficient and the fourth-order term dominates. The fourth-order term constitutes the so-called background dissipation. For an equal stabilization effect, it diffuses the solution less than a second-order term. Therefore it is

used in smooth regions of the flow. In shock regions, the fourth-order dissipation has to be switched off since it causes wiggles and the second-order dissipation is to be used to eliminate wiggles.

Therefore the second-order dissipation is called the shock dissipation.

At solid boundaries, the dissipative terms in (4.22) in the direction normal to the boundary are to be set equal to zero. In the foregoing definition of the dissipative terms (4.22, 4.23) the so-called second-order and fourth-order terms only correspond to second-order derivatives and fourth-order derivatives on a smooth grid.

However, the expressions (4.22, 4.23) do not have to be changed on an irregular grid. First, they are not meant to simulate a physical viscosity. Second, they are also meant to eliminate spurious modes, i.e. the non-physical solutions of the discretization. Figure 4.10 shows the perturbation patterns in fluxes, and as a consequence also independent variables, not detected by the central type flux balance for quadrilateral and triangular grids.

Authors using Jameson‘s Runge-Kutta scheme often have their variant of the dissipative term. Also very often, the dissipative correction in the second to fourth step is taken to be the same as in the first step.

A formulation of the artificial viscosity applicable to unstructured grids, which is a slight extension of the formulation given by Jameson and Mavriplis, is given hereafter.

The time-step limit is calculated from (for CFL = 1)

$$\Delta t = \frac{\Omega_i}{\sum_e (|V_n| + c)\Delta s}$$

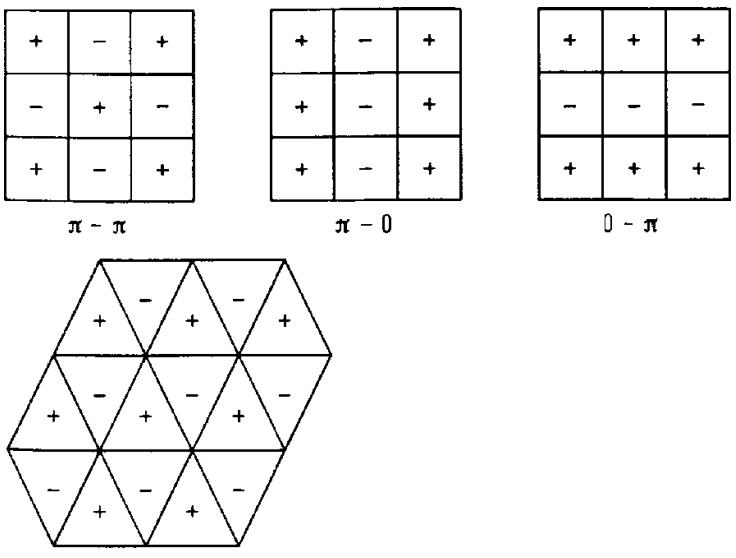

Fig. 4.10 Spurious modes for cell-centered central discretization where the subscript I denotes

the node, Vn is the normal velocity on an edge, obtained by

averaging, c is the velocity of sound obtained similarly, and Δs is the length of the edge. Ωi is the volume and the summation is taken over all edges.

The second-order smoothing operator is then, similar to (4.23), obtained by a sum of terms:

$$\varepsilon_{i,j}^{(2)}\,\sigma_{i,j}(U_j - U_i)$$

Where the subscript j denotes the surrounding nodes. The weight function εi,j is obtained from

$$\varepsilon_{i,j}^{(2)} = \kappa^{(2)}\max(\nu_i, \nu_j)$$

where νi and νj are pressure switches. The pressure switch νi is defined by

$$\nu_i = \frac{\mathrm{abs}\{\sum_j (p_j - p_i)\}}{\sum_j (p_j + p_i)}$$

$\sigma_{i,j}$ is a scaling factor given by

$$\sigma_{i,j} = \max\left(\frac{\Omega_i}{\Delta t}, \frac{\Omega_j}{\Delta t}\right)$$

With Δt the time step obtained from (4.24) for CFL = 1.

To define the fourth-order smoothing, first un-weighted pseudo-Laplacians are constructed by

$$\Delta U_i = \sum_j (U_j - U_i)$$

The fourth-order term is then given by a sum of terms:

$$\varepsilon_{i,j}^{(4)}\sigma_{i,j}(\Delta U_j - \Delta U_i)$$

Where

$$\varepsilon_{i,j}^{(4)} = \max(0, \kappa^{(4)} - \varepsilon_{i,j}^{(2)})$$

The scaling factors $\sigma_{i,j}$ allow the writing of the effective flux through a cell-face as

$$F_{i,j} - D_{i,j}$$

Where Fi,j is the physical flux and Di,j is the dissipation term, given by

$$D_{i,j} = \sigma_{i,j}[\varepsilon^{(2)}_{i,j}(U_j - U_i) - \varepsilon^{(4)}_{i,j}(\Delta U_j - \Delta U_i)]$$

The resulting flux (4.26) usually is called a numerical flux.