Chapter 2
Non-dissipative Core Scheme of CESE Method

This chapter is devoted to demonstrating the basic ideas in the CESE method. These ideas include the adoption of a space–time integral form of governing equations as the starting point of scheme construction, as well as the introduction of conservation element (CE) and solution element (SE) in the discretization of space–time domain. Then, the non-dissipative core scheme of the CESE method will be presented in detail.

2.1 Space–Time Integral Form of Governing Equations

Governing equations for a specific physical problem can be expressed in both differential and integral forms. Usually, a differential equation or a set of differential equations can clearly describe the evolution of a physical system. The differential forms of governing equations are prevalent in textbooks and theoretical research works, due to their compactness in writing and the maturity in the mathematical analysis on differential equations.

In the area of numerical simulation, the finite difference method is directly applied to the differential equations, while the finite volume method and finite element method require the governing equations to be cast into integral forms before numerical treatments. In fact, the performance of a numerical method will be influenced by the form of equations that is used in the numerical method, even though different forms of governing equations can be mathematically equivalent. As will be shown in this book, a major feature of the CESE method is the adoption of a space–time integral form of the governing equations, in which time and space are treated on the same footing.

For illustrative purposes, we consider the compressible Euler equations for 2D planar flows, which can be written in a differential form as

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$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{0}, \tag{2.1}$$

where $\boldsymbol{U}$ denotes the vector of conserved variables such that

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \end{pmatrix}, \tag{2.2}$$

where $\boldsymbol{F}$ and $\boldsymbol{G}$ are the inviscid fluxes of the form

$$\mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E + p)u \end{pmatrix}, \ \mathbf{G} = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E + p)v \end{pmatrix} \tag{2.3}$$

In Eqs. (2.2) and (2.3), ρ is the density of the fluid, u and v are the x-component and y-component of the flow velocity, respectively, p is the static pressure, and E is the total energy per unit volume of the fluid. Note that once the equation of state (EOS) is provided, Eq. (2.1) becomes a closed set of equations. Here, flux vectors $\boldsymbol{F}$ and $\boldsymbol{G}$ are regarded as functions of conserved vector $\boldsymbol{U}$. A set of equations in the form of Eq. (2.1) is called a system of conservation laws.

By using the gradient operator in 2D physical space

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right), \tag{2.4}$$

Equation (2.1) can also be written in a divergence form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{H} = \mathbf{0}, \tag{2.5}$$

where $\boldsymbol{H}$ is a matrix composed of spatial flux vectors $\boldsymbol{F}$ and $\boldsymbol{G}$:

$$\mathbf{H} = (\mathbf{F}, \mathbf{G}) \tag{2.6}$$

Therefore, the divergence form of Euler equation states that at time t and point (x, y), the temporal rate of change of conserved quantities plus the divergence of the spatial flux of these quantities must be zero.

Consider a control volume denoted by V in 2D physical space, as shown in Fig. 2.1, with the surface $S(V)$ and the unit outward normal vector $\boldsymbol{n}$ on the surface. Integrating Eq. (2.5) over the control volume V and applying the Gauss's theorem, one obtains

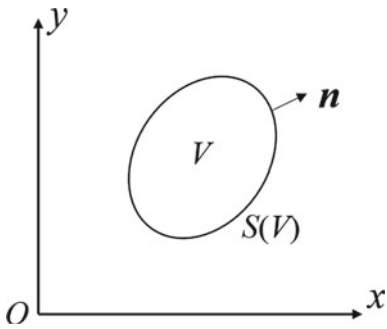

Fig. 2.1 Schematic of a control volume in two-dimensional physical space

$$\frac{\partial}{\partial t}\left(\int_V \mathbf{U}\,\mathrm{d}V\right)+\oint_{S(V)}\mathbf{H}\cdot\mathbf{n}\,\mathrm{d}S=\mathbf{0}, \tag{2.7}$$

which can be interpreted as follows: the temporal rate of change of conserved quantities within the volume V must equal to the net inward flow rate of these quantities through the surface $S(V)$. This integral form of Euler Eq. (2.7) is the starting point of the well-known finite volume method (FVM) in computational fluid dynamics.

With a unified treatment of time and physical space, we can define x, y, and t as coordinates in a three-dimensional Euclidean space, called the space–time domain. On this basis, the definition of gradient operator can be extended as

$$\nabla\equiv\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y},\frac{\partial}{\partial t}\right) \tag{2.8}$$

and Eq. (2.1) can be written in a divergence-free form as

$$\nabla\cdot\mathbf{h}=\mathbf{0}, \tag{2.9}$$

where the matrix $\boldsymbol{h}$ is composed of both flux vectors and the conserved vector $\boldsymbol{U}$:

$$\mathbf{h}=(\mathbf{F},\mathbf{G},\mathbf{U}) \tag{2.10}$$

By applying Gauss's theorem to the integration of Eq. (2.9) over an arbitrary control volume V in the 3D space–time domain as shown in Fig. 2.2, the Euler equation is eventually formulated as

$$\oint_{S(V)}\mathbf{h}\cdot\mathbf{n}\,\mathrm{d}S=\mathbf{0} \tag{2.11}$$

which means the balancing of flux is enforced for a space–time control volume. Clearly, this equation gives a direct description of the space–time conservation of mass, momentum, and energy in fluid flows, which faithfully preserves the original physical laws.

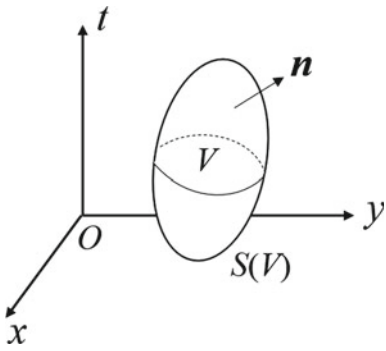

Fig. 2.2 Schematic of a control volume in three-dimensional space–time domain

Equation (2.11) provides an example of the space–time integral form of governing equations for physical problems. It is worth noting that the space–time integral form and the traditional integral form like Eq. (2.7) state the same physics and must be equivalent to each other in mathematics, but they can lead to different numerical schemes. In contrast to the finite volume method, the CESE method numerically implements the space–time integral form of governing equations, emphasizing on the conservative property in the unity of time and physical space.

2.2 Definitions of Conservation Elements and Solution Elements

The CESE method starts with discretizing the space–time domain which is relevant to the computation. The discretization procedure generates the mesh for the physical space and determines the time-step size for the time-marching algorithm, similar to most CFD methods. The features of the CESE discretization include the construction of control volumes for the space–time integral form of the governing equation, the arrangement of the solution points, and the selection of the unknown variables to be calculated and stored at each solution point. All these features can be demonstrated by introducing two special concepts: the conservation element (CE) and the solution element (SE), which coin the algorithm accordingly.

To explain the CESE method in a simple way, we begin with the application of the CESE method to a 1D scalar conservation law of the form, without loss of generality

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0. \tag{2.12}$$

With a uniform division of the 1D physical space and a constant time step, the space–time mesh is constructed as a 2D x–t plane as shown in Fig. 2.3 (solid lines). The spatial coordinate of the j-th mesh node is denoted by x_j, with the corresponding cell centre position at $x_{j+1/2} = (x_j + x_{j+1})/2$, and the cell size of $\Delta x = x_{j+1} - x_j$. In this

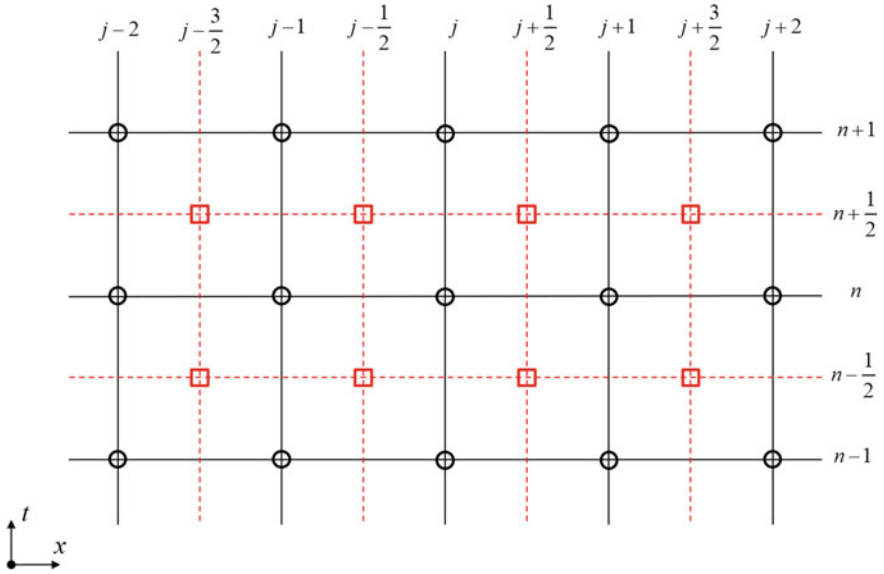

Fig. 2.3 Mesh and arrangement of solution points for 1D CESE scheme

time-marching algorithm, each step between t_{n-1} and t_n consists of two half steps: $[t_{n-1}, t_{n-1/2}]$ and $[t_{n-1/2}, t_n]$, with the time-step size of $\Delta t = t_n - t_{n-1}$.

The unknown function $u(x, t)$ is represented by the discrete values of u at a set of specific space–time points, called solution points which are shown as mesh nodes in Fig. 2.3—black circles for integer time levels $\{t_0, t_1, \ldots, t_n, \ldots\}$ and red squares (cell centres) for half-integer time levels $\{t_{1/2}, t_{3/2}, \ldots, t_{n+1/2}, \ldots\}$. In other words, a staggered mesh is used at each intermediate time level. In the CESE scheme, both the unknown variable u and its spatial derivative u_x will be calculated and stored at each solution point (e.g. point (j, n)):

$$u_j^n \equiv u(x_j, t_n),\ (u_x)_j^n \equiv \frac{\partial u}{\partial x}\left(x_j, t_n\right) \tag{2.13}$$

The paths of information flow in a single CESE time step is illustrated in the schematic diagram in Fig. 2.4. As seen, a highly compact stencil in space and time is used in the CESE scheme. If a half time step it is treated as the basic iteration, the halfwidth of the symmetric stencil is then $\Delta x/2$ and unknowns at point (j, n) only depend on the data stored at $(j - 1/2, n - 1/2)$ and $(j + 1/2, n - 1/2)$.

Based on the space–time mesh shown in Fig. 2.3, a set of small space–time elements, named conservation elements (CE), can be constructed, as demonstrated in Fig. 2.5. A CE is assigned to each solution point. For example, $(\mathrm{CE})_j^n$ is denoted as the CE for point (j, n), which is the rectangle with four vertices at the points $(j - 1/2, n - 1/2)$, $(j + 1/2, n - 1/2)$, $(j + 1/2, n)$, and $(j - 1/2, n)$. Apparently, the CEs cover the whole space–time domain without overlap. It is noteworthy that

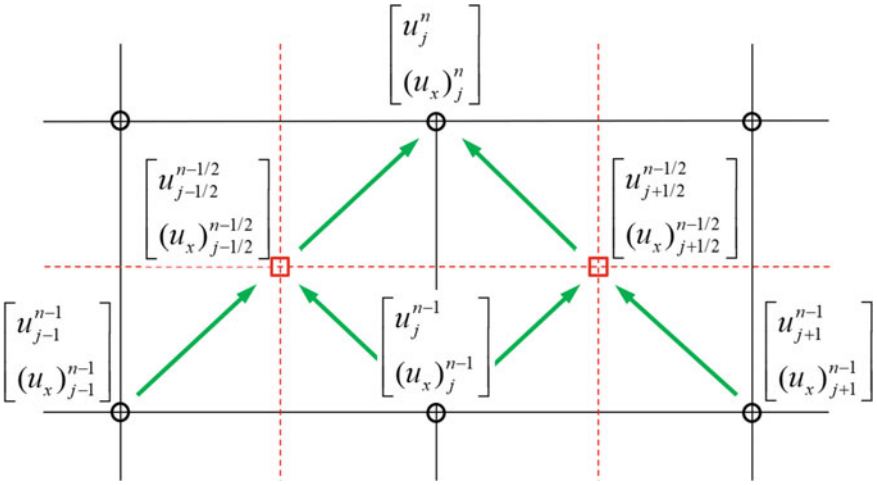

Fig. 2.4 The information flow in one CESE time step with time-marching variables

the arrangement of CEs is staggered in two successive half time steps. Accordingly, the space–time integral form of Eq. (2.12) is numerically implemented within each conservation element and discrete equations for unknowns are established.

When performing the space–time integration of Eq. (2.12) over a CE, an important question arises: how to evaluate u and f along the boundary of the CE. This leads to the

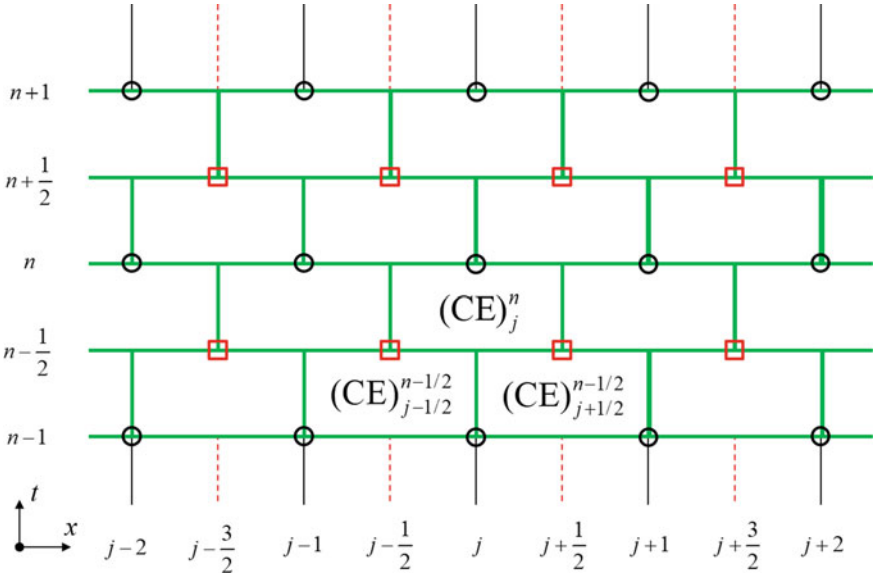

Fig. 2.5 Schematic of conservation elements (CEs) arrangement

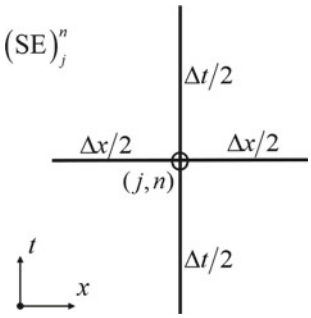

Fig. 2.6 Schematic of the solution element (SE) associated with solution point (j, n)

introduction of a solution element (SE) for each solution point, as shown in Fig. 2.6. $(\mathrm{SE})_j^n$ composed of two line segments bisecting each other at point (j, n), forming a cross with four endpoints $(j + 1/2, n)$, $(j, n + 1/2)$, $(j - 1/2, n)$, and $(j, n - 1/2)$. For half-integer points, SEs can be defined in the same way. Note that conservation element $(\mathrm{CE})_j^n$ is bounded by line segments belonging to three solution elements: $(\mathrm{SE})_j^n$, $(\mathrm{SE})_{j-1/2}^{n-1/2}$, and $(\mathrm{SE})_{j+1/2}^{n-1/2}$. In the CESE scheme, the functions $u(x, t)$ and f (x, t) are assumed to be linear along each line segment of a SE and are approximated by first-order Taylor expansions about the centre of the SE. Specifically, in the solution element $(\mathrm{SE})_j^n$, u and f are constructed as

$$u(x,t) = u_j^n + (u_x)_j^n(x - x_j) + (u_t)_j^n(t - t_n),\ (x,t) \in (\mathrm{SE})_j^n \tag{2.14}$$

$$f(x,t) = f_j^n + (f_x)_j^n(x - x_j) + (f_t)_j^n(t - t_n),\ (x,t) \in (\mathrm{SE})_j^n \tag{2.15}$$

where u_t and f_t are the temporal derivatives of u and f, respectively.

2.3 Non-dissipative Core Scheme: a Scheme

In this section, we present a non-dissipative CESE scheme, named the a scheme, to solve the 1D scalar conservation law, Eq. (2.12). A space–time flux vector is defined as

$$\mathbf{h} = (f, u) \tag{2.16}$$

where f and u can be regarded as the components of flux vector $\boldsymbol{h}$ in x-direction and t-direction, respectively. According to this definition, Eq. (2.12) can be converted into the space–time integral form of Eq. (2.11) by following the procedure in Sect. 2.1.

Consider a half step marching from time level $n-1/2$ to time level n. At the solution point (j, n), two independent unknowns u_j^n and $(u_x)_j^n$, need to be calculated simultaneously. Therefore, two algebraic equations need to be formulated by discretizing

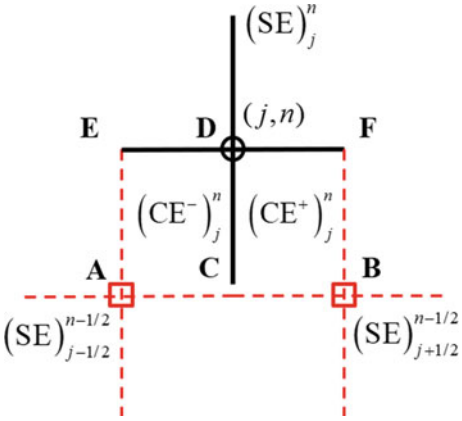

Fig. 2.7 Definition of sub-CEs: CE^- and CE^+, and the associated SEs

the integral conservation law. For this purpose, the conservation element $(CE)_j^n$ is split into two sub-elements: $(CE^-)_j^n$ and $(CE^+)_j^n$. As shown in Fig. 2.7, $(CE^-)_j^n$ and $(CE^+)_j^n$ are the rectangle ACDE and the rectangle CBFD, respectively. Each edge of these rectangles belongs to one of the three SEs associated with $(CE)_j^n$.

Next, the space–time integral conservation law is implemented over each of the sub-CEs. Let the control volume V in Eq. (2.11) be $(CE^-)_j^n$ and $(CE^+)_j^n$ in turn, one can obtain

$$\oint_{S(CE^-);} \mathbf{h} \cdot \mathbf{n} \mathrm{dS} = 0 \tag{2.17}$$

and

$$\oint_{S(\mathrm{CE}^+)_j^n} \mathbf{h} \cdot \mathbf{n} \, \mathrm{d}S = 0, \tag{2.18}$$

where $\boldsymbol{h}$ is the space–time flux vector expressed in Eq. (2.16) and $\boldsymbol{n}$ is the unit outward normal vector on the boundary of $(CE^-)_j^n$ or $(CE^+)_j^n$.

As depicted in Fig. 2.8, the average values of $u(x, t)$ on line segments DE, DF, AC, and BC are denoted by $U_L{}^*$, $U_R{}^*$, U_L, and U_R, respectively, while the average values of $f\ (x, t)$ on line segments AE, BF, and CD are presented by F_L, F_R, and F_C, respectively. Notably, CD is the interface between two sub-CEs. With this notation, integral Eqs. (2.17) and (2.18) can be expressed as

$$U_L^* \frac{\Delta x}{2} = U_L \frac{\Delta x}{2} + (F_L - F_C) \frac{\Delta t}{2}, \tag{2.19}$$

$$U_R^* \frac{\Delta x}{2} = U_R \frac{\Delta x}{2} + (F_C - F_R) \frac{\Delta t}{2}, \tag{2.20}$$

which explicitly state the balance of space–time flux in each sub-CE.

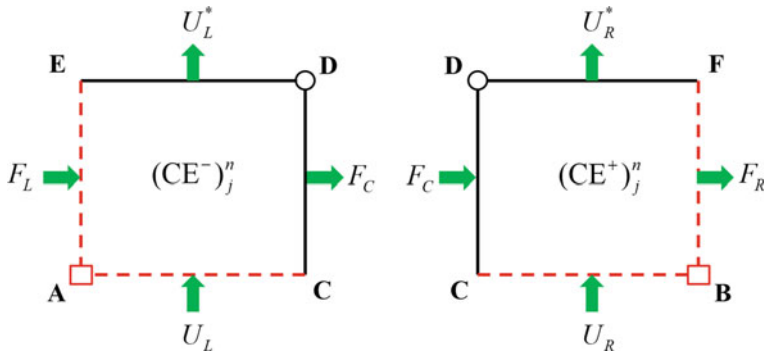

Fig. 2.8 Space–time flux through the each boundary of sub-CEs

To proceed with the scheme construction, the time-marching variables (i.e. u and u_x) at the solution points will be linked with $U_L{}^*$, $U_R{}^*$, U_L, U_R, F_L, F_R, and F_C in Eqs. (2.19) and (2.20), using the concept of the solution element. Recall that u and f can be calculated by first-order Taylor expansions about the solution point, by assuming them to be linear functions of x and t inside each individual SE. Since line segments AC and AE belong to $(\mathrm{SE})_{j-1/2}^{n-1/2}$, U_L and F_L can be obtained in terms of the known information stored at $(j-1/2, n-1/2)$, i.e., point A in Fig. 2.8. Performing Taylor expansions in $(\mathrm{SE})_{j-1/2}^{n-1/2}$ yields

$$U_L = u_{j-1/2}^{n-1/2} + \frac{\Delta x}{4}(u_x)_{j-1/2}^{n-1/2}, \tag{2.21}$$

$$F_L = f_{j-1/2}^{n-1/2} + \frac{\Delta t}{4}(f_t)_{j-1/2}^{n-1/2} \tag{2.22}$$

Similarly, because BC and BF belong to $(\mathrm{SE})_{j+1/2}^{n-1/2}$, U_R and F_R can be obtained by the Taylor expansions about solution point $(j+1/2, n-1/2)$:

$$U_R = u_{j+1/2}^{n-1/2} - \frac{\Delta x}{4}(u_x)_{j+1/2}^{n-1/2} \tag{2.23}$$

$$F_R = f_{j+1/2}^{n-1/2} + \frac{\Delta t}{4}(f_t)_{j+1/2}^{n-1/2} \tag{2.24}$$

In Eqs. (2.21)–(2.24), u and u_x at time level $n-1/2$ are the known values. In addition, since $f = f(u)$ is a prescribed function in the conservation law,

$$f_{j\pm1/2}^{n-1/2} = f(u_{j\pm1/2}^{n-1/2}) \tag{2.25}$$

By applying the chain rule, the spatial derivative of f is described as

$$(f_x)_{j\pm1/2}^{n-1/2} = \left[\left(\partial f \big/ \partial u\right)u_x\right]_{j\pm1/2}^{n-1/2} \tag{2.26}$$

The temporal derivative of u can be obtained using Eq. (2.12),

$$(u_t)_{j\pm1/2}^{n-1/2} = -(f_x)_{j\pm1/2}^{n-1/2} \tag{2.27}$$

By applying the chain rule again, the temporal derivative of f is derived as

$$(f_t)_{j\pm1/2}^{n-1/2} = \left[\left(\partial f \big/ \partial u\right)u_t\right]_{j\pm1/2}^{n-1/2} \tag{2.28}$$

Accordingly, U_L, F_L, U_R, and F_R can be explicitly calculated using the above formulas.

The first-order Taylor expansion in $(\mathrm{SE})_j^n$ is used again to relate ${U_L}^*$ and ${U_R}^*$ to unknowns u_j^n and $(u_x)_j^n$ at time level n:

$$U_L^* = u_j^n - \frac{\Delta x}{4}(u_x)_j^n \tag{2.29}$$

$$U_R^* = u_j^n + \frac{\Delta x}{4}(u_x)_j^n \tag{2.30}$$

Substituting Eqs. (2.29) and (2.30) into (2.19) and (2.20) yields

$$u_j^n - \frac{\Delta x}{4}(u_x)_j^n = U_L + (F_L - F_C)\frac{\Delta t}{\Delta x}, \tag{2.31}$$

$$u_j^n + \frac{\Delta x}{4}(u_x)_j^n = U_R + (F_C - F_R)\frac{\Delta t}{\Delta x} \tag{2.32}$$

Adding Eqs. (2.31)–(2.32), one can derive

$$u_j^n = \frac{1}{2}(U_L + U_R) + \frac{\Delta t}{2\Delta x}(F_L - F_R) \tag{2.33}$$

and subtracting Eqs. (2.31) from (2.32), one has

$$\frac{\Delta x}{4}(u_x)_j^n = \frac{1}{2}(U_R - U_L) + \frac{\Delta t}{2\Delta x}(2F_C - F_L - F_R) \tag{2.34}$$

Up to now, Eq. (2.33) is presented as an explicit time-marching formula for u_j^n, but $(u_x)_j^n$ still cannot be directly calculated by Eq. (2.34). The reason is because F_C, which presents the average value of flux f through the interface CD, has not been addressed. In the original CESE scheme, F_C is provided by the Taylor expansion in $(\mathrm{SE})_j^n$, i.e.,

$$F_C = f_j^n - \frac{\Delta t}{4}(f_t)_j^n \tag{2.35}$$

With a similar procedure to Eqs. (2.25)–(2.28), f_j^n and $(f_t)_j^n$ can be expressed in terms of u_j^n and $(u_x)_j^n$. Since u_j^n is determined by Eq. (2.33), a time-marching formula for the only unknown in Eq. (2.34), $(u_x)_j^n$, can eventually be derived.

Note that a complete CESE time step consists of two half steps: a half step marching from nodes to centres and another half step marching from centres to nodes. The marching schemes for both half steps are identical, except for the indexes of the solution points. Usually, the initial conditions of u and u_x are specified at the initial time, $t_0 = 0$ and the corresponding boundary conditions for u and u_x need to be implemented at the boundaries of x.

The above CESE scheme is referred to as the *a* scheme [1] in the literature. Define a solution vector

$$\mathbf{q}_j^n = \begin{bmatrix} u_j^n \\ \dfrac{\Delta x}{4}(u_x)_j^n \end{bmatrix}, \tag{2.36}$$

and let function $f\ (u)$ be a linear one:

$$f = au,\ a \text{ is a constant} \tag{2.37}$$

The *a* scheme, which is mainly expressed by Eqs. (2.33) and (2.34), can then be rewritten in a matrix form:

$$\mathbf{q}_j^n = \mathbf{Q}_L \mathbf{q}_{j-1/2}^{n-1/2} + \mathbf{Q}_R \mathbf{q}_{j+1/2}^{n-1/2} \tag{2.38}$$

where the coefficient matrices are

$$\mathbf{Q}_L = \frac{1}{2}\begin{bmatrix} 1+\nu & 1-\nu^2 \\ -1 & -1+\nu \end{bmatrix},\ \mathbf{Q}_R = \frac{1}{2}\begin{bmatrix} 1-\nu & -1+\nu^2 \\ 1 & -1-\nu \end{bmatrix} \tag{2.39}$$

and ν is a constant, which is defined as

$$\nu \equiv a\frac{\Delta t}{\Delta x} \tag{2.40}$$

Analogously, we apply Eq. (2.38) to the half-step marching from time level $n-1$ to time level $n-1/2$, and obtain

$$\mathbf{q}_{j-1/2}^{n-1/2} = \mathbf{Q}_L \mathbf{q}_{j-1}^{n-1} + \mathbf{Q}_R \mathbf{q}_j^{n-1}, \tag{2.41}$$

$$\mathbf{q}_{j+1/2}^{n-1/2} = \mathbf{Q}_L \mathbf{q}_j^{n-1} + \mathbf{Q}_R \mathbf{q}_{j+1}^{n-1}, \tag{2.42}$$

After substituting Eqs. (2.41) and (2.42) into (2.38), a complete time step in the a scheme can be formulated as.

$$\mathbf{q}_j^n = (\mathbf{Q}_L)^2 \mathbf{q}_{j-1}^{n-1} + (\mathbf{Q}_L \mathbf{Q}_R + \mathbf{Q}_R \mathbf{Q}_L)\mathbf{q}_j^{n-1} + (\mathbf{Q}_R)^2 \mathbf{q}_{j+1}^{n-1}. \tag{2.43}$$

In fact, the numerical dissipation, dispersion, and stability of different CESE schemes can be conveniently analysed using their matrix forms like Eq. (2.43).

An unique feature of this a scheme is its use of Taylor expansion in the inverse time direction, to relate the interface flux F_C to the marching variables (see Eq. (2.35)). Such a treatment makes the a scheme the space–time inversion invariant and renders this scheme non-dissipative [2]. From a historical perspective, the a scheme forms the non-dissipative core of subsequent CESE-family schemes.

The a scheme described in this chapter is restricted to 1D scalar problems and uniform meshes. First-order Taylor expansions are used in each solution element in the present scheme. Since the a scheme is reversible in time, it cannot be used for practical applications, considering that real physical processes are irreversible in time to respect the second law of thermodynamics. Accordingly, substantial improvements have been made to develop this a scheme into a viable numerical method. In Chap. 3, we will describe different approaches to introducing necessary numerical dissipation into the CESE scheme, which result in two categories of CESE schemes: the central CESE schemes and the upwind CESE schemes. In Chap. 4, we will describe the extensions of CESE schemes to multi-dimensional Cartesian and unstructured computational meshes. In Chap. 5, high-order Taylor expansions in solution elements will be used to achieve high-order accuracy in both space and time, without enlarging the spatial stencil or adding time-integration stages.

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