



The $\alpha(4)$ Scheme—A High Order Neutrally Stable CESE Solver

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Abstract

The CESE development is driven by a belief that a solver should (i) enforce conservation laws in both space and time, and (ii) be built from a non-dissipative (i.e., neutrally stable) core scheme so that the numerical dissipation can be controlled effectively. To provide a solid foundation for a systematic CESE development of high order schemes, in this paper we describe a new high order (4-5th order) and neutrally stable CESE solver of the advection equation $\partial u/\partial t + a\partial u/\partial x = 0$. The space-time stencil of this two-level explicit scheme is formed by one point at the upper time level and two points at the lower time level. Because it is associated with four independent mesh variables u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ (the numerical analogues of u , $\partial u/\partial x$, $\partial^2 u/\partial x^2$, and $\partial^3 u/\partial x^3$, respectively) and four equations per mesh point, the new scheme is referred to as the $a(4)$ scheme. As in the case of other similar CESE neutrally stable solvers, the $a(4)$ scheme enforces conservation laws in space-time locally and globally, and it has the basic, forward marching, and backward marching forms. Assuming $|\nu| \neq 3$ ($\nu \stackrel{\text{def}}{=} a\Delta t/\Delta x$), these forms are equivalent and satisfy a space-time inversion (STI) invariant property which is shared by the advection equation. Based on the concept of STI invariance, a set of algebraic relations is developed and used to prove that the $a(4)$ scheme must be neutrally stable when it is stable. Numerically, it has been established that the scheme is stable if $|\nu| < 1/3$.

1. Introduction

The space-time conservation element and solution element (CESE) method is a high-resolution and genuinely multidimensional method for solving conservation laws [1–73]. Its nontraditional features include: (i) a unified treatment of space and time; (ii) the introduction of conservation elements (CEs) and solution elements (SEs) as the vehicles for enforcing space-time flux conservation; (iii) a novel time marching strategy that has a space-time staggered stencil at its core and, as such, fluxes at an interface can be evaluated without using any interpolation or extrapolation procedure (which, in turn, leads to the method's ability to capture shocks without using Riemann solvers); (iv) the requirement that each scheme be built from a non-dissipative core scheme and, as a result, the numerical dissipation can be controlled effectively; and (v) the fact that mesh values of the physical dependent variables and their spatial derivatives are considered as independent marching variables to be solve for simultaneously.

Without using flux-splitting or other special techniques, since its inception in 1991 [1] the unstructured-mesh compatible CESE method has been used to obtain numerous accurate 1D, 2D and 3D steady and unsteady flow solutions with Mach numbers ranging from 0.0028 to 10 [51]. The physical phenomena modeled include traveling and interacting shocks, acoustic waves, vortex shedding, viscous flows, detonation waves, cavitation, flows in fluid film bearings, heat conduction with melting and/or freezing, electrodynamics, MHD vortex, hydraulic jump, crystal growth, and chromatographic problems [3–73]. In particular, the rather unique capability of the CESE method to resolve both strong shocks and small disturbances (e.g., acoustic waves) simultaneously [13,15,16] makes it an effective tool for attacking computational aeroacoustics (CAA) problems. Note that the fact that second-order CESE schemes can solve CAA problems accurately is an exception to the commonly-held belief that a second-order scheme is not adequate for solving CAA problems. Also note that, while numerical dissipation is needed for shock capturing, it may also result in annihilation of small disturbances. Thus a solver that can handle both strong shocks and small disturbances simultaneously must be able to overcome this difficulty.

In spite of its nontraditional features and potent capabilities, the core ideas of the CESE method are simple. In fact, all of its key features are the inescapable results of an honest pursuit driven by these simple ideas. The first and foremost is the belief that the method must be solid in physics. As such, in the CESE development, conservation laws are enforced locally and globally in their natural space-time unity forms for 1D, 2D and 3D cases. Moreover, because *direct* physical interaction generally occurs only among the immediate neighbors, use of the simplest stencil also becomes a CESE requirement. Obviously, this requirement is also very helpful in simplifying boundary-condition implementation.

The second idea is derived from the realization that stability and accuracy are two competing issues in time-accurate computations, i.e., too much numerical dissipation would degrade accuracy while too little of it will cause instability. In other words, to meet both accuracy and stability requirements, computation must be performed away from the edge (“cliff”) of instability but not too far from it. This represents a real dilemma in numerical method development. As an example, schemes with high-order accuracy generally has high accuracy and low numerical dissipation. However, it is susceptible to instability. In fact, in dealing with complicated real-world problems, stability of these schemes often is difficult to maintain without resorting to ad hoc treatments. To confront this issue head-on, in CESE development, it is required that a solver be built from a non-dissipative (i.e., neutrally stable) core scheme. By definition, computations involving a neutrally stable scheme are performed right on the edge of instability and therefore the numerical results generated are non-dissipative. As such numerical dissipation can be controlled effectively if the deviation of a solver from its non-dissipative core scheme can be adjusted using some built-in parameters. Note that the above idea also plays an essential role in the recent successful development of a family of Courant number insensitive schemes [59,61,64,65,67].

Other CESE ideas are: (i) the flux at an interface be evaluated in a simple and consistent manner; (ii) genuinely multidimensional schemes be built as simple, consistent and straightforward extensions of 1D schemes; (iii) triangular and tetrahedral meshes be used in 2D and 3D cases, respectively, so that the method is compatible to the simplest unstructured meshes and thus can be used to solve problems with complex geometries; and (iv) logical structures and approximation techniques used be as simple as possible, and special techniques that has only limited applicability and may cause undesirable side effects be avoided. Fortunately for the CESE development, as it turns out, the realization of the above lesser ideas (i)–(iv) follows effortlessly from that of the first two core ideas.

The first model equation considered in the CESE development is the simple convection equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad (1.1)$$

where the advection speed $a \neq 0$ is a constant. Let $x_1 = x$, and $x_2 = t$ be considered as the coordinates of a two-dimensional Euclidean space E_2 . Then, because Eq. (1.1) can be expressed as $\nabla \cdot \vec{h} = 0$ with $\vec{h} \stackrel{\text{def}}{=} (au, u)$, Gauss’ divergence theorem in the space-time E_2 implies that Eq. (1.1) is the differential form of the integral conservation law

$$\oint_{S(V)} \vec{h} \cdot d\vec{s} = 0 \quad (1.2)$$

As depicted in Fig. 1, here (i) $S(V)$ is the boundary of an arbitrary *space-time* region V in E_2 , and (ii) $d\vec{s} = d\sigma \vec{n}$ with $d\sigma$ and \vec{n} , respectively, being the area and the unit outward normal vector of a surface element on $S(V)$. Note that: (i) because $\vec{h} \cdot d\vec{s}$ is the *space-time* flux of \vec{h} leaving the region V through the surface element $d\vec{s}$, Eq. (1.2) simply states that the total *space-time* flux of \vec{h} leaving V through $S(V)$ vanishes; (ii) in E_2 , $d\sigma$ is the length of a line segment on the simple closed curve $S(V)$; and (iii) all mathematical operations can be carried out as though E_2 were an ordinary two-dimensional Euclidean space.

It is well known that a solution to Eq. (1.1) represents *non-dissipative* data propagation along its characteristic lines defined by $dx/dt = a$. Moreover, Eq. (1.1) is invariant under space-time inversion (STI), i.e., it transforms back to itself if x and t are replaced by $-x$ and $-t$, respectively. (In physics, STI invariance generally is referred to as *PT* invariance where *P* denotes a mirror-image or spatial-reflection operation while *T* denotes a time-reversal operation). Thus a solution to Eq. (1.1) possesses the following properties: (i) it

is completely determined by the data specified at an initial time level; (ii) its value at a space-time point has a finite domain of dependence (a point) at the initial time level; and (iii) the space-time inversion image of a solution to Eq. (1.1) is also a solution and vice versa. As such, in the initial CESE development, the focus is on the construction of an ideal core solver of Eq. (1.1) that enforces the conservation law Eq. (1.2) and also possesses all other properties of Eq. (1.1), i.e., it is a two-level, explicit, non-dissipative, and STI invariant solver. An in-depth account of this development and the resulting “ a ” scheme is given in [71]. As it turns out, the 2nd-order accurate a scheme (i) has a space-time stencil formed by one mesh point at the upper time level and two mesh points at the lower time level; and (ii) it is neutrally stable if $\nu^2 < 1$ where $\nu = a\Delta t/\Delta x$. Also, at each space-time mesh point (j, n) , the a scheme is associated with two independent mesh variables u_j^n and $(u_x)_j^n$ (the numerical analogues of u and $\partial u/\partial x$, respectively) and two equations.

Until recently, with one exception (a three-level and 3rd-order accurate scheme reported on p. 80 of [1]), all CESE solvers of Eq. (1.1) are two-level and 2nd-order accurate extensions of the a scheme. To initiate a systematic development of CESE schemes with high order accuracy, two new high order accurate, conservation-law enforcing, and neutrally stable CESE solvers of Eq. (1.1) has been developed recently. Both solvers are explicit and involving two time levels. The space-time stencil of one of them is formed by one point at the upper time level and three points at the lower time level. Because it is associated with three independent mesh variables u_j^n , $(u_x)_j^n$ and $(u_{xx})_j^n$ (the numerical analogues of u , $\partial u/\partial x$, and $\partial^2 u/\partial x^2$, respectively) and three equations per mesh point, the scheme is referred to as the $a(3)$ scheme in [72]. On the other hand, the space-time stencil of the second scheme to be described here is formed by one point at the upper time level and only two points at the lower time level. Because it is associated with four independent mesh variables u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ (the numerical analogues of u , $\partial u/\partial x$, $\partial^2 u/\partial x^2$, and $\partial^3 u/\partial x^3$, respectively) and four equations per mesh point, hereafter the new scheme is referred to as the $a(4)$ scheme.

2. The $a(4)$ scheme

To proceed, consider the set Ω_1 of space-time staggered mesh points (j, n) (dots in Fig. 2(a)), where

$$\Omega_1 \stackrel{\text{def}}{=} \{(j, n) | j, n = 0, \pm 1, \pm 2, \pm 3, \dots, \text{ and } (j + n) \text{ is an odd integer}\} \quad (2.1)$$

Each $(j, n) \in \Omega_1$ is associated with a solution element, i.e., $\text{SE}(j, n)$ (see Fig. 2(b)). Let points H , G , L , and M (marked by small open circles in Figs. 2(b)–2(f)) be the midpoints of the line segments \overline{AF} , \overline{AC} , \overline{AI} , and \overline{AK} , respectively. Then, by definition, $\text{SE}(j, n)$ is the *interior* of the *space-time* region bounded by a dashed curve depicted in Fig. 2(b). It includes a horizontal line segment \overline{ED} , a vertical line segment \overline{BJ} , two inclining line segments \overline{HL} and \overline{GM} , and their immediate neighborhood.

At this juncture, the reader is warned that the notation used here may differ from that used in previous CESE papers [1-70]. In particular, (i) the mesh indices j and n are only allowed to be whole integers here; and (ii) the spatial and temporal intervals that are denoted by $\Delta x/2$ and $\Delta t/2$, respectively, in [1-70] are denoted by Δx and Δt , respectively, here. These changes are introduced so that the $a(4)$ scheme can be compared with the $a(3)$ scheme on the same footing. Note that the $a(3)$ scheme, like most established schemes, is constructed over a set of mesh points which are *not* staggered in space-time.

Let $(x, t) \in \text{SE}(j, n)$. Then Eqs. (1.1) and (1.2) will be simulated numerically assuming that $u(x, t)$ and $\vec{h}(x, t)$, respectively, are approximated by

$$\begin{aligned} u^*(x, t; j, n) &\stackrel{\text{def}}{=} u_j^n + (u_x)_j^n(x - x_j) + (u_t)_j^n(t - t^n) + \frac{1}{2}(u_{xx})_j^n(x - x_j)^2 + (u_{xt})_j^n(x - x_j)(t - t^n) \\ &\quad + \frac{1}{2}(u_{tt})_j^n(t - t^n)^2 + \frac{1}{6}(u_{xxx})_j^n(x - x_j)^3 + \frac{1}{2}(u_{xxt})_j^n(x - x_j)^2(t - t^n) \\ &\quad + \frac{1}{2}(u_{xtt})_j^n(x - x_j)(t - t^n)^2 + \frac{1}{6}(u_{ttt})_j^n(t - t^n)^3 \end{aligned} \quad (2.2)$$

and

$$\vec{h}^*(x, t; j, n) \stackrel{\text{def}}{=} (au^*(x, t; j, n), u^*(x, t; j, n)) \quad (2.3)$$

Note that: (i) u_j^n , $(u_x)_j^n$, $(u_t)_j^n$, $(u_{xx})_j^n$, $(u_{xt})_j^n$, $(u_{tt})_j^n$, $(u_{xxx})_j^n$, $(u_{xxt})_j^n$, $(u_{xtt})_j^n$, and $(u_{ttt})_j^n$ are constants in $SE(j, n)$, and the numerical analogues of the values of u , $\partial u/\partial x$, $\partial u/\partial t$, $\partial^2 u/\partial x^2$, $\partial^2 u/\partial x \partial t$, $\partial^2 u/\partial t^2$, $\partial^3 u/\partial x^3$, $\partial^3 u/\partial x^2 \partial t$, $\partial^3 u/\partial x \partial t^2$, and $\partial^3 u/\partial t^3$ at the mesh point (j, n) , respectively; (ii) (x_j, t^n) are the coordinates of the mesh point (j, n) where $x_j = j\Delta x$ and $t^n = n\Delta t$; (iii) $u^*(x, t; j, n)$ represents a 3rd-order Taylor's approximation of u ; and (iv) Eq. (2.3) is the numerical analogy of the definition $\vec{h} = (au, u)$.

For any $(j, n) \in \Omega_1$, let $u = u^*(x, t; j, n)$ satisfy Eq. (1.1) for all $(x, t) \in SE(j, n)$. Then one has

$$\begin{aligned} (u_t)_j^n &= -a(u_x)_j^n, & (u_{xt})_j^n &= -a(u_{xx})_j^n, & (u_{tt})_j^n &= a^2(u_{xx})_j^n, \\ (u_{xxt})_j^n &= -a(u_{xxx})_j^n, & (u_{xtt})_j^n &= a^2(u_{xxx})_j^n, & (u_{ttt})_j^n &= -a^3(u_{xxx})_j^n \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.4)$$

Substituting Eq. (2.4) into Eq. (2.2), one has

$$\begin{aligned} u^*(x, t; j, n) &= u_j^n + (u_x)_j^n [(x - x_j) - a(t - t^n)] + \frac{1}{2}(u_{xx})_j^n [(x - x_j) - a(t - t^n)]^2 \\ &\quad + \frac{1}{6}(u_{xxx})_j^n [(x - x_j) - a(t - t^n)]^3 \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.5)$$

i.e., u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ are the only independent mesh variables associated with (j, n) .

With the above preliminaries, next we describe the basic form of the $a(4)$ scheme.

2.1. The basic form of the $a(4)$ scheme

Let E_2 be divided into non-overlapping space-time triangular regions (see Fig. 2(a)) referred to as conservation elements (CEs). As depicted in Figs. 2(c)–2(f), (i) each $(j, n) \in \Omega_1$ is assigned with four CEs, i.e., $CE(j, n; \ell)$, $\ell = 1, 2, 3, 4$; (ii) each CE represents a right triangle with the end points of its hypotenuse $\in \Omega_1$ but not the third vertex; and (iii) the space-time E_2 can be filled by $CE(j, n; \ell)$, $\ell = 1, 2, 3, 4$; and $(j, n) \in \Omega_1$. The $a(4)$ scheme will be constructed by assuming that the flux of \vec{h}^* conserves over CEs, i.e.,

$$\oint_{S(CE(j, n; \ell))} \vec{h}^* \cdot d\vec{s} = 0, \quad \ell = 1, 2, 3, 4; (j, n) \in \Omega_1 \quad (2.6)$$

Using the special case $\ell = 1$ as an example, how Eq. (2.6) can be turned into a set of relations linking the mesh variables at two diagonally opposite neighboring mesh points will be explained step-by-step in the following remarks:

- (a) By definition, on $S(CE(j, n; 1))$ (i.e., the boundary of $CE(j, n; 1)$), the line segments \overline{AD} and \overline{AG} belong to $SE(j, n)$ while \overline{CD} and \overline{CG} belong to $SE(j+1, n-1)$. Note that, strictly speaking, points D and G do not belong to either $SE(j, n)$ or $SE(j+1, n-1)$. This fact, however, does not pose a problem for flux evaluation over $S(CE(j, n; 1))$ because the values of \vec{h}^* at isolated points do not contribute to the flux of \vec{h}^* over a finite line segment.
- (b) The straight line passing through points A and C can be defined by

$$t = t^n - \frac{\Delta t}{\Delta x}(x - x_j) \quad \text{or} \quad t = t^{n-1} - \frac{\Delta t}{\Delta x}(x - x_{j+1}) \quad (2.7)$$

- (c) For $CE(j, n; 1)$, the outward unit normal vectors \vec{n} on \overline{AD} , \overline{CD} , and \overline{AC} are

$$\vec{n}_1 \stackrel{\text{def}}{=} (0, 1), \quad \vec{n}_2 \stackrel{\text{def}}{=} (1, 0), \quad \text{and} \quad \vec{n}_3 \stackrel{\text{def}}{=} -\frac{(\Delta t, \Delta x)}{\sqrt{(\Delta t)^2 + (\Delta x)^2}} \quad (2.8)$$

respectively.

- (d) Obviously, (i) the length of the line segment joining any two neighboring points (x, t^n) and $(x + dx, t^n)$ on \overline{AD} is $d\sigma = |dx|$; and (ii) the length of the line segment joining any two neighboring points (x_{j+1}, t) and $(x_{j+1}, t + dt)$ on \overline{CD} is $d\sigma = |dt|$.

On the other hand, because $|dt/dx| = \Delta t/\Delta x$ for any two neighboring points (x, t) and $(x + dx, t + dt)$ on \overline{AC} , the length of the line segment joining these two points is

$$d\sigma \stackrel{\text{def}}{=} \sqrt{(dt)^2 + (dx)^2} = \sqrt{(\Delta t)^2 + (\Delta x)^2} \cdot (|dx|/\Delta x) \quad (2.9)$$

- (e) With the aid of (i) Eq. (2.3), (ii) the preliminaries given in the above items (c) and (d), and (iii) the relation $d\vec{s} = d\sigma \vec{n}$, one concludes that, for $\text{CE}(j, n; 1)$,

$$\vec{h}^* \cdot d\vec{s} = \begin{cases} u^*|dx| & \text{on } \overline{AD} \\ au^*|dt| & \text{on } \overline{CD} \\ -(1 + \nu)u^*|dx| & \text{on } \overline{AC} \end{cases} \quad (2.10)$$

Here $\nu \stackrel{\text{def}}{=} a\Delta t/\Delta x$ is the Courant number.

- (f) With the aid of Eq. (2.10) and the comments made in the above items (a) and (b), one can see that, for the case $\ell = 1$, Eq. (2.6) \Leftrightarrow

$$\begin{aligned} & \int_{x_j}^{x_{j+1}} u^*(x, t^n; j, n) dx + \int_{t^{n-1}}^{t^n} au^*(x_{j+1}, t; j + 1, n - 1) dt \\ & - (1 + \nu) \int_{x_j}^{x_{j+1/2}} u^*\left(x, t^n - \frac{\Delta t}{\Delta x}(x - x_j); j, n\right) dx \quad (j, n) \in \Omega_1 \quad (2.11) \\ & - (1 + \nu) \int_{x_{j+1/2}}^{x_{j+1}} u^*\left(x, t^{n-1} - \frac{\Delta t}{\Delta x}(x - x_{j+1}); j + 1, n - 1\right) dx = 0 \end{aligned}$$

where (i) the symbol “ \Leftrightarrow ” is used as a shorthand for the statement “if and only if”, and (ii) $x_{j+1/2} \stackrel{\text{def}}{=} x_j + (\Delta x/2)$.

- (g) Let

$$(u_{\bar{x}})_j^n \stackrel{\text{def}}{=} \frac{\Delta x}{2} (u_x)_j^n, \quad (u_{\bar{x}\bar{x}})_j^n \stackrel{\text{def}}{=} \frac{(\Delta x)^2}{4} (u_{xx})_j^n, \quad \text{and} \quad (u_{\bar{x}\bar{x}\bar{x}})_j^n \stackrel{\text{def}}{=} \frac{(\Delta x)^3}{8} (u_{xxx})_j^n, \quad (j, n) \in \Omega_1 \quad (2.12)$$

Then, with the aid of Eq. (2.12), the expression obtained by substituting Eq. (2.5) into (2.11) can be cast into the following form:

$$\begin{aligned} & (1 - \nu) \left[u + \frac{\nu + 3}{2} u_{\bar{x}} + \frac{\nu^2 + 4\nu + 7}{6} u_{\bar{x}\bar{x}} + \frac{(\nu + 3)(\nu^2 + 2\nu + 5)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = (1 - \nu) \left[u - \frac{3\nu + 1}{2} u_{\bar{x}} + \frac{7\nu^2 + 4\nu + 1}{6} u_{\bar{x}\bar{x}} - \frac{(3\nu + 1)(5\nu^2 + 2\nu + 1)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n-1} \quad (j, n) \in \Omega_1 \quad (2.13) \end{aligned}$$

To simplify notation, in the above and hereafter we adopt a convention that can be explained using an expression on the left side of Eq. (2.13) as an example, i.e.,

$$\begin{aligned} & \left[u + \frac{\nu + 3}{2} u_{\bar{x}} + \frac{\nu^2 + 4\nu + 7}{6} u_{\bar{x}\bar{x}} + \frac{(\nu + 3)(\nu^2 + 2\nu + 5)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = u_j^n + \frac{\nu + 3}{2} (u_{\bar{x}})_j^n + \frac{\nu^2 + 4\nu + 7}{6} (u_{\bar{x}\bar{x}})_j^n + \frac{(\nu + 3)(\nu^2 + 2\nu + 5)}{24} (u_{\bar{x}\bar{x}\bar{x}})_j^n \end{aligned}$$

Similarly, for the cases $\ell = 2, 3, 4$, Eq. (2.6) implies that

$$\begin{aligned} & (1 - \nu) \left[u + \frac{3\nu + 1}{2} u_{\bar{x}} + \frac{7\nu^2 + 4\nu + 1}{6} u_{\bar{x}\bar{x}} + \frac{(3\nu + 1)(5\nu^2 + 2\nu + 1)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = (1 - \nu) \left[u - \frac{\nu + 3}{2} u_{\bar{x}} + \frac{\nu^2 + 4\nu + 7}{6} u_{\bar{x}\bar{x}} - \frac{(\nu + 3)(\nu^2 + 2\nu + 5)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n-1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.14)$$

$$\begin{aligned} & (1 + \nu) \left[u + \frac{\nu - 3}{2} u_{\bar{x}} + \frac{\nu^2 - 4\nu + 7}{6} u_{\bar{x}\bar{x}} + \frac{(\nu - 3)(\nu^2 - 2\nu + 5)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = (1 + \nu) \left[u - \frac{3\nu - 1}{2} u_{\bar{x}} + \frac{7\nu^2 - 4\nu + 1}{6} u_{\bar{x}\bar{x}} - \frac{(3\nu - 1)(5\nu^2 - 2\nu + 1)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n-1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.15)$$

and

$$\begin{aligned} & (1 + \nu) \left[u + \frac{3\nu - 1}{2} u_{\bar{x}} + \frac{7\nu^2 - 4\nu + 1}{6} u_{\bar{x}\bar{x}} + \frac{(3\nu - 1)(5\nu^2 - 2\nu + 1)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = (1 + \nu) \left[u - \frac{\nu - 3}{2} u_{\bar{x}} + \frac{\nu^2 - 4\nu + 7}{6} u_{\bar{x}\bar{x}} - \frac{(\nu - 3)(\nu^2 - 2\nu + 5)}{24} u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n-1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.16)$$

respectively.

At this juncture, note that:

(a) Because

$$\frac{\partial u}{\partial \bar{x}} = \frac{\Delta x}{2} \frac{\partial u}{\partial x}, \quad \frac{\partial^2 u}{\partial \bar{x}^2} = \frac{(\Delta x)^2}{4} \frac{\partial^2 u}{\partial x^2}, \quad \text{and} \quad \frac{\partial^3 u}{\partial \bar{x}^3} = \frac{(\Delta x)^3}{8} \frac{\partial^3 u}{\partial x^3} \quad \text{if} \quad \bar{x} \stackrel{\text{def}}{=} \frac{x}{\Delta x/2}$$

the normalized parameters $(u_{\bar{x}})_j^n$, $(u_{\bar{x}\bar{x}})_j^n$, and $(u_{\bar{x}\bar{x}\bar{x}})_j^n$ can be interpreted as the numerical analogues of the values at (j, n) of the first, second, and third derivatives of u with respect to the normalized coordinate \bar{x} .

(b) Note that: (i) the vector \vec{h}^* at any *horizontal* or *vertical* interface separating two neighboring CEs is evaluated using the information from a single SE; (ii) the vector \vec{h}^* at one half of any *inclining* interface separating two neighboring CEs is evaluated using the information from a single SE while that at another half is evaluated using the information from another SE; and (iii) the unit outward normal vector on the surface element pointing outward from one of two neighboring CEs sharing the same element is exactly the negative of that pointing outward from another CE. Thus one concludes that the flux leaving one of the two neighboring CEs through the interface they share is the negative of that leaving another CE through the same interface. Due to this interface flux cancelation and the fact that the CEs are nonoverlapping and can fill the space-time E_2 , the local conservation relations Eq. (2.6) lead to a global conservation relation, i.e., *the total flux of \vec{h}^* leaving the boundary of any space-time region that is the union of any combination of CEs vanishes.*

Let $1 - \nu \neq 0$ and $1 + \nu \neq 0$, i.e.,

$$\nu^2 \neq 1 \quad (2.17)$$

Then Eqs. (2.13)–(2.16) can be simplified by eliminating (i) the common factors $(1 - \nu)$ on the both sides of each of Eqs. (2.13) and (2.14); and (ii) the common factors $(1 + \nu)$ on the both sides of each of Eqs. (2.15) and (2.16). By adding the simplified forms of Eqs. (2.13) and (2.14) together and then subtracting one of them from another, one has

$$\begin{aligned} & \left[u + (1 + \nu) u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3} u_{\bar{x}\bar{x}} + \frac{(1 + \nu)(1 + \nu^2)}{3} u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = \left[u - (1 + \nu) u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3} u_{\bar{x}\bar{x}} - \frac{(1 + \nu)(1 + \nu^2)}{3} u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n-1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.18)$$

and

$$\left[u_{\bar{x}} + (1+\nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 + 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \left[u_{\bar{x}} - (1+\nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 + 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n-1}, \quad (j, n) \in \Omega_1 \quad (2.19)$$

Note that Eq. (2.19) has been further simplified by eliminating the common factors $(1 - \nu)$ which appear on the both sides of the original subtraction result. Similarly, the simplified forms of Eqs. (2.15) and (2.16) imply that

$$\begin{aligned} & \left[u - (1 - \nu)u_{\bar{x}} + \frac{2(1 - \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} - \frac{(1 - \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ &= \left[u + (1 - \nu)u_{\bar{x}} + \frac{2(1 - \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{(1 - \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n-1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.20)$$

and

$$\left[u_{\bar{x}} - (1-\nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 - 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \left[u_{\bar{x}} + (1-\nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 - 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n-1}, \quad (j, n) \in \Omega_1 \quad (2.21)$$

Note that Eqs. (2.18) and (2.19) are stricter than Eqs. (2.13) and (2.14) in the sense that the former imply the latter for any ν but the latter imply the former only if an extra condition (i.e., $1 - \nu \neq 0$ for this case) is imposed. Similarly, Eqs. (2.20) and (2.21) are stricter than Eqs. (2.15) and (2.16). Hereafter, by definition, the system of equations formed by Eqs. (2.18)–(2.21) is referred to as the basic form of the $a(4)$ scheme. In the following, we derive the forward marching form.

2.2. The forward marching form of the $a(4)$ scheme

To simply notation, temporally the expressions on the right sides of Eqs. (2.18)–(2.21) will be denoted by s_1 , s_2 , s_3 , and s_4 , respectively. Then, by adding Eqs. (2.18) and (2.20) together and then subtracting one of them from another, one has

$$\left[u + \nu u_{\bar{x}} + \frac{2(1 + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{\nu(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \frac{1}{2}(s_1 + s_3), \quad (j, n) \in \Omega_1 \quad (2.22)$$

and

$$\left[u_{\bar{x}} + \frac{2\nu}{3}u_{\bar{x}\bar{x}} + \frac{1 + \nu^2}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \frac{1}{2}(s_1 - s_3), \quad (j, n) \in \Omega_1 \quad (2.23)$$

In turn, by subtracting Eq. (2.23) from both Eqs. (2.19) and (2.21), one has

$$\left(\frac{\nu + 3}{3} \right) \left[u_{\bar{x}\bar{x}} + \frac{3\nu + 1}{4}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = s_2 - \frac{1}{2}(s_1 - s_3), \quad (j, n) \in \Omega_1 \quad (2.24)$$

and

$$\left(\frac{\nu - 3}{3} \right) \left[u_{\bar{x}\bar{x}} + \frac{3\nu - 1}{4}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = s_4 - \frac{1}{2}(s_1 - s_3), \quad (j, n) \in \Omega_1 \quad (2.25)$$

Let $\nu - 3 \neq 0$ and $\nu + 3 \neq 0$, i.e.,

$$\nu^2 \neq 9 \quad (2.26)$$

Then Eqs. (2.24) and (2.25) \Leftrightarrow

$$(u_{\bar{x}\bar{x}\bar{x}})_j^n = \frac{6s_2}{\nu + 3} - \frac{6s_4}{\nu - 3} + \frac{18(s_1 - s_3)}{\nu^2 - 9}, \quad (j, n) \in \Omega_1 \quad (2.27)$$

and

$$(u_{\bar{x}\bar{x}})_j^n = -\frac{3(3\nu-1)s_2}{2(\nu+3)} + \frac{3(3\nu+1)s_4}{2(\nu-3)} - \frac{15\nu(s_1-s_3)}{\nu^2-9}, \quad (j, n) \in \Omega_1 \quad (2.28)$$

Next, by substituting Eqs. (2.27) and (2.28) into Eq. (2.23), one has

$$(u_{\bar{x}})_j^n = \frac{(\nu+1)(\nu-2)s_2}{\nu+3} - \frac{(\nu-1)(\nu+2)s_4}{\nu-3} + \frac{3(3\nu^2-7)(s_1-s_3)}{2(\nu^2-9)}, \quad (j, n) \in \Omega_1 \quad (2.29)$$

Finally, by substituting Eqs. (2.27)–(2.29) into Eq. (2.22), one arrives at

$$u_j^n = \frac{(3\nu-1)s_2}{\nu+3} - \frac{(3\nu+1)s_4}{\nu-3} + \frac{1}{2} \left[1 - \frac{\nu(\nu^2-29)}{\nu^2-9} \right] s_1 + \frac{1}{2} \left[1 + \frac{\nu(\nu^2-29)}{\nu^2-9} \right] s_3, \quad (j, n) \in \Omega_1 \quad (2.30)$$

Hereafter, in Eqs. (2.27)–(2.30) and all other equations derived from them, Eq. (2.26) will be assumed implicitly.

To proceed, let

$$\vec{q}(j, n) \stackrel{\text{def}}{=} \begin{pmatrix} u_j^n \\ (u_{\bar{x}})_j^n \\ (u_{\bar{x}\bar{x}})_j^n \\ (u_{\bar{x}\bar{x}\bar{x}})_j^n \end{pmatrix} \quad (j, n) \in \Omega_1 \quad (2.31)$$

$$\vec{s}_+ \stackrel{\text{def}}{=} \begin{pmatrix} s_1 \\ s_2 \end{pmatrix} \quad \text{and} \quad \vec{s}_- \stackrel{\text{def}}{=} \begin{pmatrix} s_3 \\ s_4 \end{pmatrix} \quad (2.32)$$

$$C_+(\nu) \stackrel{\text{def}}{=} \begin{pmatrix} 1 & -(1+\nu) & (2/3)(1+\nu+\nu^2) & -(1+\nu)(1+\nu^2)/3 \\ 0 & 1 & -(1+\nu) & (7\nu^2+10\nu+7)/12 \end{pmatrix} \quad (2.33)$$

$$C_-(\nu) \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 1-\nu & (2/3)(1-\nu+\nu^2) & (1-\nu)(1+\nu^2)/3 \\ 0 & 1 & 1-\nu & (7\nu^2-10\nu+7)/12 \end{pmatrix} \quad (2.34)$$

$$D_+(\nu) \stackrel{\text{def}}{=} \begin{pmatrix} \{1 - [\nu(\nu^2-29)/(\nu^2-9)]\}/2 & (3\nu-1)/(\nu+3) \\ (3/2)(3\nu^2-7)/(\nu^2-9) & (\nu+1)(\nu-2)/(\nu+3) \\ -15\nu/(\nu^2-9) & -(3/2)(3\nu-1)/(\nu+3) \\ 18/(\nu^2-9) & 6/(\nu+3) \end{pmatrix} \quad (2.35)$$

and

$$D_-(\nu) \stackrel{\text{def}}{=} \begin{pmatrix} \{1 + [\nu(\nu^2-29)/(\nu^2-9)]\}/2 & -(3\nu+1)/(\nu-3) \\ -(3/2)(3\nu^2-7)/(\nu^2-9) & -(\nu-1)(\nu+2)/(\nu-3) \\ 15\nu/(\nu^2-9) & (3/2)(3\nu+1)/(\nu-3) \\ -18/(\nu^2-9) & -6/(\nu-3) \end{pmatrix} \quad (2.36)$$

Then: (i) by the definition of s_1 , s_2 , s_3 , and s_4 , one has

$$\vec{s}_+ = C_+(\nu) \vec{q}(j+1, n-1) \quad \text{and} \quad \vec{s}_- = C_-(\nu) \vec{q}(j-1, n-1), \quad (j, n) \in \Omega_1 \quad (2.37)$$

and (ii) Eqs. (2.27)–(2.30) can be cast into the form

$$\vec{q}(j, n) = D_+(\nu) \vec{s}_+ + D_-(\nu) \vec{s}_-, \quad (j, n) \in \Omega_1 \quad (2.38)$$

By substituting Eqs. (2.37) into (2.38), Eqs. (2.27)–(2.30) can be cast into the matrix form

$$\vec{q}(j, n) = Q_+(\nu) \vec{q}(j+1, n-1) + Q_-(\nu) \vec{q}(j-1, n-1), \quad (j, n) \in \Omega_1 \quad (2.39)$$

where

$$Q_+(\nu) \stackrel{\text{def}}{=} D_+(\nu) C_+(\nu) \quad \text{and} \quad Q_-(\nu) \stackrel{\text{def}}{=} D_-(\nu) C_-(\nu) \quad (2.40)$$

Hereafter the system of equations formed by Eqs. (2.27)–(2.30) or its equivalent Eq. (2.39) is referred to as the forward marching form of the $a(4)$ scheme. According to the above derivation, the forward marching form is a result of the basic form and the assumption Eq. (2.26). Also note that here Eq. (2.40) is cast into a form different from the forward marching form of the a scheme (e.g., Eq. (3.48) in [71]), i.e., *the symbols $Q_+(\nu)$ and $Q_-(\nu)$ used in the a scheme are replaced in the $a(4)$ scheme by $Q_-(\nu)$ and $Q_+(\nu)$, respectively.*

As a preliminary to a later development, next we will take a side tour and introduce the concept of invariance under space-time inversion.

2.3. Invariance under space-time inversion

Let $u = u(x, t)$ be a solution to Eq. (1.1) in the domain $-\infty < x, t < +\infty$, i.e.,

$$\frac{\partial u(x, t)}{\partial t} + a \frac{\partial u(x, t)}{\partial x} \equiv 0, \quad -\infty < x, t < +\infty \quad (2.41)$$

Let

$$x' \stackrel{\text{def}}{=} -x \quad \text{and} \quad t' \stackrel{\text{def}}{=} -t \quad (2.42)$$

and

$$\hat{u}(x, t) \stackrel{\text{def}}{=} u(-x, -t) \quad (2.43)$$

Then (i) Eq. (2.41) \Leftrightarrow

$$\frac{\partial u(x', t')}{\partial t'} + a \frac{\partial u(x', t')}{\partial x'} \equiv 0, \quad -\infty < x', t' < +\infty \quad (2.44)$$

and (ii)

$$\frac{\partial}{\partial t'} = -\frac{\partial}{\partial t} \quad \text{and} \quad \frac{\partial}{\partial x'} = -\frac{\partial}{\partial x} \quad (2.45)$$

Thus one concludes that Eq. (2.41) \Leftrightarrow

$$\frac{\partial \hat{u}(x, t)}{\partial t} + a \frac{\partial \hat{u}(x, t)}{\partial x} \equiv 0, \quad -\infty < x, t < +\infty \quad (2.46)$$

In other words, if $u = u(x, t)$ is a solution to Eq. (1.1), so must be $u = \hat{u}(x, t)$ and vice versa. Because the one-to-one mapping

$$(x, t) \leftrightarrow (-x, -t), \quad -\infty < x, t < +\infty \quad (2.47)$$

represents a space-time inversion (STI) operation, hereafter (i) a pair of functions such as u and \hat{u} will be referred to as the STI images of each other; and (ii) a partial differential equation (PDE) such as Eq. (1.1) is said to be STI invariant if the STI image of a solution is also a solution and vice versa.

Next let

$$u^{(k, \ell)}(x, t) \stackrel{\text{def}}{=} \frac{\partial^{k+\ell} u(x, t)}{\partial x^k \partial t^\ell} \quad \text{and} \quad \hat{u}^{(k, \ell)}(x, t) \stackrel{\text{def}}{=} \frac{\partial^{k+\ell} \hat{u}(x, t)}{\partial x^k \partial t^\ell}, \quad -\infty < x, t < +\infty; \quad k, \ell = 0, 1, 2, \dots \quad (2.48)$$

Then, with the aid of the chain rule, Eqs. (2.42), (2.43), and (2.48) imply that

$$\begin{aligned} \hat{u}^{(k, \ell)}(x, t) &= \frac{\partial^{k+\ell} u(-x, -t)}{\partial x^k \partial t^\ell} = (-1)^{k+\ell} \frac{\partial^{k+\ell} u(x', t')}{\partial x'^k \partial t'^\ell} \quad -\infty < x, t < +\infty; \quad k, \ell = 0, 1, 2, \dots \\ &= (-1)^{k+\ell} u^{(k, \ell)}(x', t') = (-1)^{k+\ell} u^{(k, \ell)}(-x, -t) \end{aligned} \quad (2.49)$$

i.e.,

$$\hat{u}^{(k, \ell)}(x, t) = \begin{cases} u^{(k, \ell)}(-x, -t) & \text{if } (k + \ell) \text{ is even} \\ -u^{(k, \ell)}(-x, -t) & \text{if } (k + \ell) \text{ is odd} \end{cases} \quad (2.50)$$

According to Eq. (2.48), $u^{(0,0)} = u$ and $\hat{u}^{(0,0)} = \hat{u}$. Thus Eq. (2.43) is a special case of Eq. (2.49) with $k = \ell = 0$.

In the following, the concept of STI invariance will be introduced for the $a(4)$ scheme. As a preliminary, note that: (i) $(j, n) \in \Omega_1 \Leftrightarrow (-j, -n) \in \Omega_1$; (ii)

$$(j, n) \leftrightarrow (-j, -n) \quad (2.51)$$

is the numerical analogue of the STI mapping Eq. (2.47); and (iii) $u_j^n, (u_x)_j^n, (u_t)_j^n, (u_{xx})_j^n, (u_{xt})_j^n, (u_{tt})_j^n, (u_{xxx})_j^n, (u_{xxt})_j^n, (u_{xtt})_j^n$, and $(u_{ttt})_j^n$ are the numerical analogues of the values of $u, \partial u/\partial x, \partial u/\partial t, \partial^2 u/\partial x^2, \partial^2 u/\partial x \partial t, \partial^2 u/\partial t^2, \partial^3 u/\partial x^3, \partial^3 u/\partial x^2 \partial t, \partial^3 u/\partial x \partial t^2$, and $\partial^3 u/\partial t^3$ at the mesh point (j, n) , respectively. Thus, motivated by Eq. (2.50), the one-to-one mapping

$$\begin{aligned} u_j^n &\leftrightarrow u_{-j}^{-n}; & (u_x)_j^n &\leftrightarrow -(u_x)_{-j}^{-n}; & (u_t)_j^n &\leftrightarrow -(u_t)_{-j}^{-n}; & (u_{xx})_j^n &\leftrightarrow (u_{xx})_{-j}^{-n} \\ (u_{xt})_j^n &\leftrightarrow (u_{xt})_{-j}^{-n}; & (u_{tt})_j^n &\leftrightarrow (u_{tt})_{-j}^{-n}; & (u_{xxx})_j^n &\leftrightarrow -(u_{xxx})_{-j}^{-n} \\ (u_{xxt})_j^n &\leftrightarrow -(u_{xxt})_{-j}^{-n}; & (u_{xtt})_j^n &\leftrightarrow -(u_{xtt})_{-j}^{-n}; & (u_{ttt})_j^n &\leftrightarrow -(u_{ttt})_{-j}^{-n} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.52)$$

is taken as the numerical analogue of the one-to-one mapping

$$u^{(k,\ell)}(x, t) \leftrightarrow \hat{u}^{(k,\ell)}(x, t), \quad -\infty < x, t < +\infty; \quad k, \ell = 0, 1, 2, 3 \quad (2.53)$$

For the independent mesh variables, by using Eq. (2.12), it is seen that the mapping Eq. (2.52) reduces to

$$\begin{pmatrix} u_j^n \\ (u_{\bar{x}})_j^n \\ (u_{\bar{x}\bar{x}})_j^n \\ (u_{\bar{x}\bar{x}\bar{x}})_j^n \end{pmatrix} \leftrightarrow \begin{pmatrix} u_{-j}^{-n} \\ -(u_{\bar{x}})_{-j}^{-n} \\ (u_{\bar{x}\bar{x}})_{-j}^{-n} \\ -(u_{\bar{x}\bar{x}\bar{x}})_{-j}^{-n} \end{pmatrix} \quad (j, n) \in \Omega_1 \quad (2.54)$$

With the aid of Eq. (2.31), Eq. (2.54) can be expressed as

$$\bar{q}(j, n) \leftrightarrow U\bar{q}(-j, -n), \quad (j, n) \in \Omega_1 \quad (2.55)$$

where

$$U \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (2.56)$$

The matrix U is unitary. In fact it is a real matrix with

$$U = U^{-1} \quad (2.57)$$

Hereafter (i) M^{-1} denotes the inverse of any nonsingular square matrix M ; (ii) for each (j, n) , $U\bar{q}(-j, -n)$ is referred to as the STI image of $\bar{q}(j, n)$; and (iii) the set formed by $U\bar{q}(-j, -n)$, $(j, n) \in \Omega_1$ is also referred to as the image of the set formed by $\bar{q}(j, n)$, $(j, n) \in \Omega_1$. According to Eq. (2.57), $\bar{q}(j, n) = UU\bar{q}(-j, -n)$. Thus $\bar{q}(j, n)$ is the STI image of $U\bar{q}(-j, -n)$ as an individual (j, n) or as the set defined over Ω_1 . In the following, we will show that the system of equations defined by each of Eqs. (2.18)–(2.21) is STI invariant, i.e., the system maps onto an equivalent system under the mapping Eq. (2.54).

As an example, consider the system defined by Eq. (2.18). Under the mapping Eq. (2.54), Eq. (2.18) maps onto

$$\begin{aligned} &\left[u - (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} - \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{-j}^{-n} \\ &= \left[u + (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{-(j+1)}^{-(n-1)} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.58)$$

At this juncture, note that, in addition to changing the sign of each $u_{\bar{x}}$ and $u_{\bar{x}\bar{x}\bar{x}}$, mapping Eq. (2.54) requires that the upper and lower indices j , n , $j + 1$, and $n - 1$ in Eq. (2.18) be replaced by their negatives, respectively. *This is different from simply replacing the symbols j and n everywhere with $-j$ and $-n$, respectively.* Moreover, to simplify argument, hereafter system B is referred to as the STI image of system A if A maps onto B under the mapping Eq. (2.54), e.g., the system Eq. (2.58) is the STI image of Eq. (2.18). Let

$$j^* \stackrel{\text{def}}{=} -j - 1 \quad \text{and} \quad n^* \stackrel{\text{def}}{=} -n + 1, \quad (j, n) \in \Omega_1 \quad (2.59)$$

Then, by using the fact that $(j^* + n^*) + (j + n) \equiv 0$ and therefore $(j^*, n^*) \in \Omega_1 \Leftrightarrow (j, n) \in \Omega_1$, Eq. (2.58) can be cast into the form

$$\begin{aligned} & \left[u + (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{j^*}^{n^*} \\ & = \left[u - (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} - \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{j^*+1}^{n^*-1} \end{aligned} \quad (j^*, n^*) \in \Omega_1 \quad (2.60)$$

By comparing Eqs. (2.18) and (2.60), one can see that the system Eq. (2.18) is identical to its STI image Eq. (2.58) (which is identical to Eq. (2.60)). Thus, under the mapping Eq. (2.54), Eq. (2.18) maps onto itself, i.e., the system Eq. (2.18) is STI invariant. QED.

The STI invariance of each of Eqs. (2.19)–(2.21) can be established in a similar manner. As such, the basic form of the $a(4)$ scheme (which is formed by all component equations in Eqs. (2.18)–(2.21)) is STI invariant.

Let $\bar{q}(j, n) = \bar{q}_o(j, n)$, $(j, n) \in \Omega_1$, be a solution to the basic form. Then, by substituting $\bar{q}(j, n) = \bar{q}_o(j, n)$ into the basic form, one obtains a system of identities involving $\bar{q}_o(j, n)$, $(j, n) \in \Omega_1$. Due to the STI invariance of the basic form, the above system of identities is equivalent to that obtained by substituting $\bar{q}(j, n) = U\bar{q}_o(-j, -n)$ into the basic form. As such $\bar{q}(j, n) = \bar{q}_o(j, n)$, $(j, n) \in \Omega_1$, represent a solution to the basic form $\Leftrightarrow \bar{q}(j, n) = U\bar{q}_o(-j, -n)$, $(j, n) \in \Omega_1$, represent another solution to the basic form. In other words, *the STI image of a solution to the basic form is also a solution and vice versa.* Obviously this conclusion is also valid for other STI invariant forms of the $a(4)$ scheme.

Next, we will establish the STI invariance of the forward marching form. As a preliminary, discussion of some basic concepts is in order. Note that for any set of variables x_ℓ, y_ℓ , $\ell = 1, 2$, the conditions

$$x_1 + y_1 = x_2 - y_2 \quad \text{and} \quad x_1 - y_1 = x_2 + y_2 \quad (2.61)$$

\Leftrightarrow

$$x_1 = x_2 \quad \text{and} \quad y_1 = -y_2 \quad (2.62)$$

Thus, the image of Eq. (2.61) under any one-to-one mapping

$$(x_\ell, y_\ell) \leftrightarrow (x'_\ell, y'_\ell), \quad \ell = 1, 2 \quad (2.63)$$

i.e.,

$$x'_1 + y'_1 = x'_2 - y'_2 \quad \text{and} \quad x'_1 - y'_1 = x'_2 + y'_2 \quad (2.64)$$

\Leftrightarrow the image of Eq. (2.62) under the same mapping, i.e.,

$$x'_1 = x'_2 \quad \text{and} \quad y'_1 = -y'_2 \quad (2.65)$$

where the variables x'_ℓ and y'_ℓ , $\ell = 1, 2$, may or may not be related to x_ℓ, y_ℓ , $\ell = 1, 2$. Moreover, in case that these two sets of variables are related, the condition Eq. (2.61) (or its equivalent Eq. (2.62)) may or may not be equivalent to the condition Eq. (2.64) (or its equivalent Eq. (2.65)). If the mapping Eq. (2.63) is such that Eq. (2.61) \Leftrightarrow the image under this mapping (i.e., Eq. (2.64)), then Eq. (2.62) (the equivalent of

Eq. (2.61) \Leftrightarrow Eq. (2.65) (the equivalent of Eq. (2.64)). Eq. (2.63) with $x'_\ell = x_\ell$ and $y'_\ell = y_\ell$, $\ell = 1, 2$, is an example of such mapping while Eq. (2.63) with $x'_\ell = y_\ell$ and $y'_\ell = x_\ell$, $\ell = 1, 2$, is not.

The STI invariance of the forward marching form will be proved assuming Eq. (2.26) (the form is undefined if Eq. (2.26) is not valid). Note that: (i) the basic form of the $a(4)$ scheme \Leftrightarrow its forward marching form for *any choice* of $\bar{q}(j, n)$, $(j, n) \in \Omega_1$; and (ii) the STI images of the basic and forward marching forms, respectively, are obtained from the basic and forward marching forms through the mapping Eq. (2.55), i.e., through replacing $\bar{q}(j, n)$ in the basic form and the forward marching form with $U\bar{q}(-j, -n)$, $(j, n) \in \Omega$. From the above observations and the illustration given in the last paragraph, one concludes that the STI image of the basic form \Leftrightarrow that of the forward marching form. Because the basic form is STI invariant, i.e., the STI image of the basic form \Leftrightarrow the basic form itself, Now we arrive at the conclusion that the forward marching form \Leftrightarrow the basic form \Leftrightarrow the STI image of the basic form \Leftrightarrow the STI image of the forward marching form. Thus the forward marching form \Leftrightarrow its STI image, i.e., the forward marching form is STI invariant. QED.

2.4. The backward marching form of the $a(4)$ scheme

According to Eq. (2.55), the STI invariance of the forward marching form implies that Eq. (2.39) \Leftrightarrow its STI image, i.e.,

$$U\bar{q}(-j, -n) = Q_+(\nu)U\bar{q}(-j-1, -n+1) + Q_-(\nu)U\bar{q}(-j+1, -n+1), \quad (j, n) \in \Omega_1 \quad (2.66)$$

By multiplying Eq. (2.66) from left using the matrix U and using Eq. (2.57), one concludes that Eq. (2.66) \Leftrightarrow

$$\bar{q}(-j, -n) = \hat{Q}_-(\nu)\bar{q}(-j-1, -n+1) + \hat{Q}_+(\nu)\bar{q}(-j+1, -n+1), \quad (j, n) \in \Omega_1 \quad (2.67)$$

where

$$\hat{Q}_-(\nu) \stackrel{\text{def}}{=} UQ_+(\nu)U \quad \text{and} \quad \hat{Q}_+(\nu) \stackrel{\text{def}}{=} UQ_-(\nu)U \quad (2.68)$$

By using Eqs. (2.33)–(2.36), (2.40), and (2.56), Eq. (2.68) implies that

$$\hat{Q}_-(\nu) = \hat{D}_+(\nu)\hat{C}_+(\nu) \quad \text{and} \quad \hat{Q}_+(\nu) = \hat{D}_-(\nu)\hat{C}_-(\nu) \quad (2.69)$$

where

$$\hat{C}_+(\nu) \stackrel{\text{def}}{=} C_+(\nu)U = \begin{pmatrix} 1 & 1+\nu & (2/3)(1+\nu+\nu^2) & (1+\nu)(1+\nu^2)/3 \\ 0 & -1 & -(1+\nu) & -(7\nu^2+10\nu+7)/12 \end{pmatrix} \quad (2.70)$$

$$\hat{C}_-(\nu) \stackrel{\text{def}}{=} C_-(\nu)U = \begin{pmatrix} 1 & -(1-\nu) & (2/3)(1-\nu+\nu^2) & -(1-\nu)(1+\nu^2)/3 \\ 0 & -1 & 1-\nu & -(7\nu^2-10\nu+7)/12 \end{pmatrix} \quad (2.71)$$

$$\hat{D}_+(\nu) \stackrel{\text{def}}{=} UD_+(\nu) = \begin{pmatrix} \{1 - [\nu(\nu^2 - 29)/(\nu^2 - 9)]\}/2 & (3\nu - 1)/(\nu + 3) \\ -(3/2)(3\nu^2 - 7)/(\nu^2 - 9) & -(\nu + 1)(\nu - 2)/(\nu + 3) \\ -15\nu/(\nu^2 - 9) & -(3/2)(3\nu - 1)/(\nu + 3) \\ -18/(\nu^2 - 9) & -6/(\nu + 3) \end{pmatrix} \quad (2.72)$$

and

$$\hat{D}_-(\nu) \stackrel{\text{def}}{=} UD_-(\nu) = \begin{pmatrix} \{1 + [\nu(\nu^2 - 29)/(\nu^2 - 9)]\}/2 & -(3\nu + 1)/(\nu - 3) \\ (3/2)(3\nu^2 - 7)/(\nu^2 - 9) & (\nu - 1)(\nu + 2)/(\nu - 3) \\ 15\nu/(\nu^2 - 9) & (3/2)(3\nu + 1)/(\nu - 3) \\ 18/(\nu^2 - 9) & 6/(\nu - 3) \end{pmatrix} \quad (2.73)$$

Next, by replacing the “dummy” indices $-j$ and $-n$ everywhere in Eq. (2.67) with j and n , respectively, and using the fact that $(-j, -n) \in \Omega_1 \Leftrightarrow (j, n) \in \Omega_1$, one can see that the system Eq. (2.67) is identical to the system

$$\bar{q}(j, n) = \hat{Q}_+(\nu)\bar{q}(j+1, n+1) + \hat{Q}_-(\nu)\bar{q}(j-1, n+1), \quad (j, n) \in \Omega_1 \quad (2.74)$$

Because the mesh variables at (j, n) can be determined in terms of those at $(j-1, n+1)$ and $(j+1, n+1)$ using Eq. (2.74), hereafter Eq. (2.74) (which is equivalent to the forward marching forms of the $a(4)$ scheme) will be referred to as the backward marching form of the $a(4)$ scheme.

Eq. (2.74) was derived using the STI invariance of the forward marching form of the $a(4)$ scheme. Alternatively, it can also be derived from the basic form. Note that: (i) by replacing the “dummy” indices j and n everywhere in Eq. (2.18) with $j - 1$ and $n + 1$ and using the fact that $(j, n) \in \Omega_1 \Leftrightarrow (j + 1, n - 1) \in \Omega_1 \Leftrightarrow (j - 1, n + 1) \in \Omega_1$, one can see that the system Eq. (2.18) is identical to the system

$$\begin{aligned} & \left[u - (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} - \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = \left[u + (1 + \nu)u_{\bar{x}} + \frac{2(1 + \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{(1 + \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n+1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.75)$$

(ii) by replacing the indices j and n everywhere in Eq. (2.19) with $j - 1$ and $n + 1$ and using the fact that $(j, n) \in \Omega_1 \Leftrightarrow (j + 1, n - 1) \in \Omega_1 \Leftrightarrow (j - 1, n + 1) \in \Omega_1$, one can see that the system Eq. (2.19) is identical to the system

$$\left[u_{\bar{x}} - (1 + \nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 + 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \left[u_{\bar{x}} + (1 + \nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 + 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_{j-1}^{n+1}, \quad (j, n) \in \Omega_1 \quad (2.76)$$

(iii) by replacing the indices j and n everywhere in Eq. (2.20) with $j + 1$ and $n + 1$ and using the fact that $(j, n) \in \Omega_1 \Leftrightarrow (j - 1, n - 1) \in \Omega_1 \Leftrightarrow (j + 1, n + 1) \in \Omega_1$, one can see that the system Eq. (2.20) is identical to the system

$$\begin{aligned} & \left[u + (1 - \nu)u_{\bar{x}} + \frac{2(1 - \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} + \frac{(1 - \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n \\ & = \left[u - (1 - \nu)u_{\bar{x}} + \frac{2(1 - \nu + \nu^2)}{3}u_{\bar{x}\bar{x}} - \frac{(1 - \nu)(1 + \nu^2)}{3}u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n+1} \end{aligned} \quad (j, n) \in \Omega_1 \quad (2.77)$$

and (iv) by replacing the indices j and n everywhere in Eq. (2.21) with $j + 1$ and $n + 1$ and using the fact that $(j, n) \in \Omega_1 \Leftrightarrow (j - 1, n - 1) \in \Omega_1 \Leftrightarrow (j + 1, n + 1) \in \Omega_1$, one can see that the system Eq. (2.21) is identical to the system

$$\left[u_{\bar{x}} + (1 - \nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 - 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_j^n = \left[u_{\bar{x}} - (1 - \nu)u_{\bar{x}\bar{x}} + \frac{7\nu^2 - 10\nu + 7}{12}u_{\bar{x}\bar{x}\bar{x}} \right]_{j+1}^{n+1}, \quad (j, n) \in \Omega_1 \quad (2.78)$$

As such Eqs. (2.75)–(2.78) are equivalent to Eqs. (2.18)–(2.21), respectively.

For each $(j, n) \in \Omega_1$, Eqs. (2.18)–(2.21) form a linear system of four equations for the four mesh variables u_j^n , $(u_{\bar{x}})_j^n$, $(u_{\bar{x}\bar{x}})_j^n$, and $(u_{\bar{x}\bar{x}\bar{x}})_j^n$. Eqs. (2.75)–(2.78) form another system. Moreover, one can see that, under the mesh variable mapping

$$\bar{q}(j, n) \leftrightarrow U\bar{q}(j, n), \quad \bar{q}(j + 1, n - 1) \leftrightarrow U\bar{q}(j - 1, n + 1) \quad \text{and} \quad \bar{q}(j - 1, n - 1) \leftrightarrow \bar{q}(j + 1, n + 1) \quad (2.79)$$

Eqs. (2.75)–(2.78), respectively, are the images of Eqs. (2.18)–(2.21) and vice versa. By using the concept introduced earlier in a discussion involving Eqs. (2.61)–(2.65), one concludes that the solution to Eqs. (2.75)–(2.78) must be the image of Eq. (2.39) (i.e., the solution to Eqs. (2.18)–(2.21)) under the mapping Eq. (2.79). In other words, the solution to Eqs. (2.75)–(2.78) is

$$U\bar{q}(j, n) = Q_+(\nu)U\bar{q}(j - 1, n + 1) + Q_-(\nu)U\bar{q}(j + 1, n + 1), \quad (j, n) \in \Omega_1 \quad (2.80)$$

By multiplying Eq. (2.80) from left using the matrix U and using Eqs. (2.57) and (2.68), one has Eq. (2.74). QED.

As a preliminary for the developments in Sec. 3, in the following, important algebraic relations involving $Q_+(\nu)$, $Q_-(\nu)$, $\hat{Q}_+(\nu)$, and $\hat{Q}_-(\nu)$ will be extracted from the STI invariance of the $a(4)$ scheme.

2.5. Algebraic relations associated with STI invariance

Let $(j_o, n_o) \in \Omega_1$ be any given fixed mesh point. Then $(j_o + 2, n_o) \in \Omega_1$ and $(j_o - 2, n_o) \in \Omega_1$. Let $\bar{q}(j_o, n_o)$, $\bar{q}(j_o + 2, n_o)$, and $\bar{q}(j_o - 2, n_o)$, respectively, be the arbitrary initial data specified at these mesh points. Let $\nu^2 \neq 9$. Then $\bar{q}(j_o + 1, n_o + 1)$ can be uniquely determined in terms of $\bar{q}(j_o, n_o)$ and $\bar{q}(j_o + 2, n_o)$ by imposing the basic form Eqs. (2.18)–(2.21) with $(j, n) = (j_o + 1, n_o + 1)$. In fact, by using the equivalent forward marching form Eq. (2.39), one has

$$\bar{q}(j_o + 1, n_o + 1) = Q_+(\nu) \bar{q}(j_o + 2, n_o) + Q_-(\nu) \bar{q}(j_o, n_o) \quad (2.81)$$

Similarly, by imposing the basic form Eqs. (2.18)–(2.21) with $(j, n) = (j_o - 1, n_o + 1)$, one has

$$\bar{q}(j_o - 1, n_o + 1) = Q_+(\nu) \bar{q}(j_o, n_o) + Q_-(\nu) \bar{q}(j_o - 2, n_o) \quad (2.82)$$

Among the conditions imposed above, (i) Eqs. (2.18) and (2.19) with $(j, n) = (j_o - 1, n_o + 1)$ represent two conditions linking $\bar{q}(j_o - 1, n_o + 1)$ and $\bar{q}(j_o, n_o)$; and (ii) Eqs. (2.20) and (2.21) with $(j, n) = (j_o + 1, n_o + 1)$ represent two conditions linking $\bar{q}(j_o + 1, n_o + 1)$ and $\bar{q}(j_o, n_o)$. Thus the four mesh variables in $\bar{q}(j_o, n_o)$ can be determined in terms of $\bar{q}(j_o + 1, n_o + 1)$ and $\bar{q}(j_o - 1, n_o + 1)$ by using the four conditions specified in the above items (i) and (ii). In fact, by using the equivalent backward marching form Eq. (2.74), one has

$$\bar{q}(j_o, n_o) = \hat{Q}_+(\nu) \bar{q}(j_o + 1, n_o + 1) + \hat{Q}_-(\nu) \bar{q}(j_o - 1, n_o + 1) \quad (2.83)$$

By substituting Eqs. (2.81) and (2.82) into (2.83), one concludes that

$$\begin{aligned} & [\hat{Q}_+(\nu)Q_-(\nu) + \hat{Q}_-(\nu)Q_+(\nu) - I] \bar{q}(j_o, n_o) \\ & + \hat{Q}_+(\nu)Q_+(\nu) \bar{q}(j_o + 2, n_o) + \hat{Q}_-(\nu)Q_-(\nu) \bar{q}(j_o - 2, n_o) = \vec{0} \end{aligned} \quad (2.84)$$

where I is the 4×4 identity matrix and $\vec{0}$ is the 4×1 null column matrix. Because Eq. (2.84) must be valid for any choice of $\bar{q}(j_o + 2, n_o)$, $\bar{q}(j_o - 2, n_o)$, and $\bar{q}(j_o, n_o)$, the coefficient matrices in front of these column matrices must vanish identically. Thus we have

$$\hat{Q}_+(\nu)Q_-(\nu) + \hat{Q}_-(\nu)Q_+(\nu) = I \quad (2.85)$$

$$\hat{Q}_+(\nu)Q_+(\nu) = \mathbf{0} \quad (2.86)$$

and

$$\hat{Q}_-(\nu)Q_-(\nu) = \mathbf{0} \quad (2.87)$$

where $\mathbf{0}$ is the 4×4 null matrix. As an example, one can prove Eq. (2.85) by substituting into Eqs. (2.84) each of the following sets of the initial data: (i) $\bar{q}(j_o + 2, n_o) = \bar{q}(j_o - 2, n_o) = 0$ and $\bar{q}(j_o, n_o) = (1, 0, 0, 0)^t$, (ii) $\bar{q}(j_o + 2, n_o) = \bar{q}(j_o - 2, n_o) = 0$ and $\bar{q}(j_o, n_o) = (0, 1, 0, 0)^t$, (iii) $\bar{q}(j_o + 2, n_o) = \bar{q}(j_o - 2, n_o) = 0$ and $\bar{q}(j_o, n_o) = (0, 0, 1, 0)^t$, and (iv) $\bar{q}(j_o + 2, n_o) = \bar{q}(j_o - 2, n_o) = 0$ and $\bar{q}(j_o, n_o) = (0, 0, 0, 1)^t$. Here \bar{c}^t denote the transpose of a 1×4 matrix \bar{c} .

Similarly, by substituting the backward marching relations

$$\bar{q}(j_o + 1, n_o - 1) = \hat{Q}_+(\nu) \bar{q}(j_o + 2, n_o) + \hat{Q}_-(\nu) \bar{q}(j_o, n_o) \quad (2.88)$$

and

$$\bar{q}(j_o - 1, n_o - 1) = \hat{Q}_+(\nu) \bar{q}(j_o, n_o) + \hat{Q}_-(\nu) \bar{q}(j_o - 2, n_o) \quad (2.89)$$

into the forward marching relation

$$\bar{q}(j_o, n_o) = Q_+(\nu) \bar{q}(j_o + 1, n_o - 1) + Q_-(\nu) \bar{q}(j_o - 1, n_o - 1) \quad (2.90)$$

one has

$$\begin{aligned} & [Q_+(\nu)\hat{Q}_-(\nu) + Q_-(\nu)\hat{Q}_+(\nu) - I]\bar{q}(j_o, n_o) \\ & + Q_+(\nu)\hat{Q}_+(\nu)\bar{q}(j_o + 2, n_o) + Q_-(\nu)\hat{Q}_-(\nu)\bar{q}(j_o - 2, n_o) = \vec{0} \end{aligned} \quad (2.91)$$

Because Eq. (2.91) must be valid for any choice of $\bar{q}(j_o + 2, n_o)$, $\bar{q}(j_o - 2, n_o)$, and $\bar{q}(j_o, n_o)$, one concludes that

$$Q_+(\nu)\hat{Q}_-(\nu) + Q_-(\nu)\hat{Q}_+(\nu) = I \quad (2.92)$$

$$Q_+(\nu)\hat{Q}_+(\nu) = \mathbf{0} \quad (2.93)$$

and

$$Q_-(\nu)\hat{Q}_-(\nu) = \mathbf{0} \quad (2.94)$$

By using Eqs. (2.57) and (2.68), it can be shown that: (i) Eq. (2.85) \Leftrightarrow Eq. (2.92) \Leftrightarrow

$$Q_-(\nu)UQ_-(\nu) + Q_+(\nu)UQ_+(\nu) = U \quad (2.95)$$

(ii) Eq. (2.86) \Leftrightarrow Eq. (2.94) \Leftrightarrow

$$Q_-(\nu)UQ_+(\nu) = \mathbf{0} \quad (2.96)$$

and (iii) Eq. (2.87) \Leftrightarrow Eq. (2.93) \Leftrightarrow

$$Q_+(\nu)UQ_-(\nu) = \mathbf{0} \quad (2.97)$$

2.6. The dual $a(4)$ scheme

In the above, the $a(4)$ schemes is defined using only the mesh points $\in \Omega_1$. Independently, it can also be defined using only the mesh points $\in \Omega_2$ where

$$\Omega_2 \stackrel{\text{def}}{=} \{(j, n) | j, n = 0, \pm 1, \pm 2, \pm 3, \dots, \text{ and } (j + n) \text{ is an even integer}\} \quad (2.98)$$

For the current 1D case where a structured mesh is used, the $a(4)$ scheme defined over Ω_1 is *completely decoupled* from that defined over Ω_2 . Thus, *there is no practical reason to carry out computations using the two decoupled schemes simultaneously.*

However, to simplify numerical comparisons between the $a(4)$ scheme and the $a(3)$ scheme which is only defined over the mesh point set

$$\Omega \stackrel{\text{def}}{=} \Omega_1 \cup \Omega_2 = \{(j, n) | j, n = 0, \pm 1, \pm 2, \dots\} \quad (2.99)$$

the numerical results to be presented in Sec. 4 are generated using the “dual” $a(4)$ scheme, i.e., the scheme formed from the two decoupled $a(4)$ schemes and defined over Ω . By the definition of STI invariance, one can see that each form of the dual $a(4)$ scheme is also STI invariant.

3. von Neumann analysis

Let $G(\nu, \theta)$ be a 4×4 nonsingular complex matrix function of ν and the phase angle θ such that

$$\bar{q}(j, n) = e^{ij\theta} [G(\nu, \theta)]^n \vec{b}, \quad (j, n) \in \Omega_1; \quad -\infty < \theta < +\infty; \quad i \equiv \sqrt{-1} \quad (3.1)$$

is a solution to Eq. (2.39) for all possible complex constant 4×1 column matrices \vec{b} . (Note: because $[G(\nu, \theta)]^n \stackrel{\text{def}}{=} \left\{ [G(\nu, \theta)]^{-1} \right\}^{|n|}$ for an integer $n < 0$, $[G(\nu, \theta)]^n$ is not defined if $n < 0$ unless $[G(\nu, \theta)]^{-1}$ exists, i.e., $G(\nu, \theta)$ is nonsingular.) By substituting Eq. (3.1) into Eq. (2.39), one has

$$[G(\nu, \theta) - e^{i\theta}Q_+(\nu) - e^{-i\theta}Q_-(\nu)] [G(\nu, \theta)]^n \vec{b} = 0, \quad n = 0, \pm 1, \pm 2, \dots \quad (3.2)$$

Because (i) $[G(\nu, \theta)]^0 = I$, and (ii) \vec{b} can be any complex constant 4×1 column matrix, Eq. (3.2) implies that

$$G(\nu, \theta) = e^{i\theta} Q_+(\nu) + e^{-i\theta} Q_-(\nu) \quad (3.3)$$

By definition, $G(\nu, \theta)$ is the amplification matrix of the forward marching form of the $a(4)$ scheme.

By using Eqs. (2.95)–(2.97), one can show easily that

$$\begin{aligned} & U [e^{i\theta} Q_-(\nu) + e^{-i\theta} Q_+(\nu)] U [e^{i\theta} Q_+(\nu) + e^{-i\theta} Q_-(\nu)] \\ &= [e^{i\theta} Q_+(\nu) + e^{-i\theta} Q_-(\nu)] U [e^{i\theta} Q_-(\nu) + e^{-i\theta} Q_+(\nu)] U = I \end{aligned} \quad (3.4)$$

Thus $G(\nu, \theta)$ defined in Eq. (3.3) is nonsingular and its inverse is

$$[G(\nu, \theta)]^{-1} = U [e^{i\theta} Q_-(\nu) + e^{-i\theta} Q_+(\nu)] U \quad (3.5)$$

Indeed, with the aid of Eq. (2.68), Eq. (3.5) is what one obtains after substituting Eq. (3.1) into the backward marching form Eq. (2.74). Moreover, by using Eqs. (2.57), (3.3), and (3.5) along with the fact that $Q_+(\nu)$ and $Q_-(\nu)$ are real matrices, one arrives at the important conclusion

$$[G(\nu, \theta)]^{-1} = U \overline{G(\nu, \theta)} U^{-1} \quad (3.6)$$

Hereafter \overline{M} denotes the complex conjugate of any matrix M .

For each (ν, θ) , the four eigenvalues $G(\nu, \theta)$ will be denoted as $\sigma_\ell(\nu, \theta)$, $\ell = 1, 2, 3, 4$, and referred to as the amplification factors of the $a(4)$ scheme. By using Eq. (3.6), next it will be shown that

$$\left\{ \frac{1}{\sigma_1(\nu, \theta)}, \frac{1}{\sigma_2(\nu, \theta)}, \frac{1}{\sigma_3(\nu, \theta)}, \frac{1}{\sigma_4(\nu, \theta)} \right\} = \left\{ \overline{\sigma_1(\nu, \theta)}, \overline{\sigma_2(\nu, \theta)}, \overline{\sigma_3(\nu, \theta)}, \overline{\sigma_4(\nu, \theta)} \right\} \quad (3.7)$$

Hereafter \bar{z} denotes the complex conjugate of any complex number z .

As a preliminary, first we introduce the following matrix theorems:

Theorem 1. Let A be a nonsingular $N \times N$ matrix with the eigenvalues λ_ℓ , $\ell = 1, 2, \dots, N$. Then (i) $\lambda_\ell \neq 0$, $\ell = 1, 2, \dots, N$; and (ii) the eigenvalues of A^{-1} are $1/\lambda_\ell$, $\ell = 1, 2, \dots, N$.

Theorem 2. Let A be a $N \times N$ matrix with the eigenvalues λ_ℓ , $\ell = 1, 2, \dots, N$. Then the eigenvalues of \overline{A} , the complex conjugate of A , are $\overline{\lambda_\ell}$, $\ell = 1, 2, \dots, N$.

Theorem 3. Let A and B be two similar $N \times N$ matrices, i.e., there exists a nonsingular $N \times N$ matrix S so that $B = S^{-1}AS$. Then A and B have the same eigenvalues, counting multiplicity.

The proof of Theorems 1 and 2 is given in Appendix A of [72] while that of Theorem 3 is given on p. 45 of [74].

To prove Eq. (3.7), consider any (ν, θ) with $\nu^2 \neq 9$. Then because the eigenvalues of the nonsingular matrix $G(\nu, \theta)$ are $\sigma_\ell(\nu, \theta)$, $\ell = 1, 2, 3, 4$, Theorem 1 implies that: (i) $\sigma_\ell(\nu, \theta) \neq 0$, $\ell = 1, 2, 3, 4$; and (ii) the eigenvalues of $[G(\nu, \theta)]^{-1}$ are $1/\sigma_\ell(\nu, \theta)$, $\ell = 1, 2, 3, 4$. Next, by using Theorems 2 and 3, and the fact that $(U^{-1})^{-1} = U$, one can see that the eigenvalues of the matrix on the right side of Eq. (3.6) are $\overline{\sigma_\ell(\nu, \theta)}$, $\ell = 1, 2, 3, 4$. Thus Eq. (3.7) now is an immediate result of Eq. (3.6). QED.

An immediate result of Eq. (3.7) is

$$\frac{1}{\sigma_1(\nu, \theta)} \cdot \frac{1}{\sigma_2(\nu, \theta)} \cdot \frac{1}{\sigma_3(\nu, \theta)} \cdot \frac{1}{\sigma_4(\nu, \theta)} = \overline{\sigma_1(\nu, \theta)} \cdot \overline{\sigma_2(\nu, \theta)} \cdot \overline{\sigma_3(\nu, \theta)} \cdot \overline{\sigma_4(\nu, \theta)}$$

i.e.,

$$|\sigma_1(\nu, \theta)| \cdot |\sigma_2(\nu, \theta)| \cdot |\sigma_3(\nu, \theta)| \cdot |\sigma_4(\nu, \theta)| = 1 \quad (3.8)$$

For any given ν , stability of the $a(4)$ scheme requires that

$$|\sigma_\ell(\nu, \theta)| \leq 1, \quad \ell = 1, 2, 3, 4 \quad (3.9)$$

Thus Eq. (3.8) implies that, for any given ν , the $a(4)$ scheme must be neutrally stable, i.e.,

$$|\sigma_\ell(\nu, \theta)| = 1, \quad \ell = 1, 2, 3, 4 \quad (3.10)$$

if it is stable. As such, Eq. (3.6) does not imply neutral stability of the $a(4)$ scheme. However, it does imply that the scheme can only be neutrally stable (i.e., non-dissipative) if it is stable. Here we have reached this conclusion without using the explicit form of $\sigma_\ell(\nu, \theta)$, $\ell = 1, 2, 3, 4$.

4. Numerical results

To assess the accuracy of the $a(4)$ scheme, consider the model problem with the PDE

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad (4.1)$$

and the exact solution

$$u = u_e(x, t) \stackrel{\text{def}}{=} \sin [2\pi(x - t)] \quad (4.2)$$

We have

$$a = \lambda = T = 1 \quad (4.3)$$

where $\lambda =$ wavelength and $T =$ period. Let (i)

$$u_{xe}(x, t) \stackrel{\text{def}}{=} \frac{\partial u_e(x, t)}{\partial x}, \quad u_{x^2e}(x, t) \stackrel{\text{def}}{=} \frac{\partial^2 u_e(x, t)}{\partial x^2}, \quad \text{and} \quad u_{x^3e}(x, t) \stackrel{\text{def}}{=} \frac{\partial^3 u_e(x, t)}{\partial x^3} \quad (4.4)$$

and (ii) the spatial domain of unit length be divided into K uniform intervals. Thus

$$\Delta x = 1/K, \quad \Delta t = \nu \Delta x \quad \text{and} \quad t = n \Delta t \quad (4.5)$$

where $n =$ number of time steps, and $t =$ total marching time.

It has been shown numerically that the $a(4)$ scheme is stable if

$$|\nu| < 1/3 \quad (4.6)$$

On the other hand, (i) the a scheme is stable if

$$|\nu| < 1 \quad (4.7)$$

and (ii) $a(3)$ scheme is stable if

$$|\nu| < 1/2 \quad (4.8)$$

In Tables 1–4, the numerical errors of several computations using the $a(4)$, $a(3)$, and a schemes are presented in terms of the parameters

$$E(K, n, \nu) \stackrel{\text{def}}{=} \sqrt{\frac{1}{K} \sum_{j=0}^{K-1} [u_j^n - u_e(x_j, t^n)]^2} \quad (4.9)$$

$$E_x(K, n, \nu) \stackrel{\text{def}}{=} \sqrt{\frac{1}{K} \sum_{j=0}^{K-1} [(u_x)_j^n - u_{xe}(x_j, t^n)]^2} \quad (4.10)$$

$$E_{xx}(K, n, \nu) \stackrel{\text{def}}{=} \sqrt{\frac{1}{K} \sum_{j=0}^{K-1} [(u_{xx})_j^n - u_{xxe}(x_j, t^n)]^2} \quad (4.11)$$

and

$$E_{xxx}(K, n, \nu) \stackrel{\text{def}}{=} \sqrt{\frac{1}{K} \sum_{j=0}^{K-1} [(u_{xxx})_j^n - u_{xxx e}(x_j, t^n)]^2} \quad (4.12)$$

The numerical errors of several simulations with $\nu = 0.1$ and $t = 9.876$ are given in Table 1. For the a scheme, as the values of K and n become larger, the values of E and E_x are both reduced by a factor of about 4 as both K and n double their values, i.e., the scheme is clearly 2nd order in accuracy for both u_j^n and $(u_x)_j^n$. For the $a(3)$ scheme, the values of E , E_x , and E_{xx} are reduced by factors of about 16, 16, and 4, respectively as both K and n double their values. Thus, for this case, the $a(3)$ scheme is 4th order in accuracy for both u_j^n and $(u_x)_j^n$ while only 2nd order in accuracy for $(u_{xx})_j^n$. On the other hand, for the $a(4)$ scheme, the values of E , E_x , E_{xx} , and E_{xxx} generally are not reduced by constant factors as both K and n double their values. However, by comparing their values before and after both K and n increase by a factor of 8, one can show that, for the $a(4)$ scheme, the estimated orders of accuracy for u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ are 4.61, 1.83, 1.61, and -0.177 , respectively.

In Table 2, the cases considered have $\nu = 0.1$ and $t = 10.00 = 10T$. For these cases where t is an integer multiple of the period T , it is seen that (i) the a scheme is again 2nd order in accuracy for both u_j^n and $(u_x)_j^n$; and (ii) the $a(3)$ scheme is 4th order in accuracy for u_j^n , $(u_x)_j^n$, and $(u_{xx})_j^n$. On the other hand, for the $a(4)$ scheme, the estimated orders of accuracy for u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ are 4.30, 2.17, 2.25 and 0.164, respectively.

In Table 3, the cases considered have $\nu = 1/3$ and $t = 9.6$. According to Eq. (4.6), $\nu = 1/3$ is right at the stability boundary of the $a(4)$ scheme. For these cases, it is seen that, aside from round-off errors, the numerical values of u_j^n and $(u_{xx})_j^n$ generated using the $a(4)$ scheme are all identical to their exact solution values, respectively. However, one observes that the round-off error for u_j^n grows linearly with n while that for $(u_{xx})_j^n$ shows signs of nonlinear growth.

In Table 4, the cases considered have $\nu = 1/3$ and $t = 10.00 = 10T$. For these cases where (i) the value of ν is right at the stability boundary of the $a(4)$ scheme and (ii) t is an integer multiple of T , aside from round-off errors, the numerical values of u_j^n , $(u_x)_j^n$, $(u_{xx})_j^n$, and $(u_{xxx})_j^n$ generated using the $a(4)$ scheme are all identical to their exact solution values, respectively. However, because of strong growth of round-off errors, these highly accurate results become unsustainable as n increases.

5. Conclusions and discussions

A thorough and rigorous discussion of a new high order neutrally stable CESE solver of Eq. (1.1) has been presented. Because this two-level explicit scheme is associated with four independent mesh variables and four equations per mesh point, it is referred to as the $a(4)$ scheme. As in the case of other similar CESE neutrally stable solvers, the $a(4)$ scheme enforces conservation laws locally and globally, and it has the basic, forward marching, and backward marching forms. Assuming $\nu^2 \neq 9$, these forms are equivalent and satisfy the STI invariant property defined in Sec. 2.

Based on the concept of STI invariance, a set of algebraic relations (Eqs. (2.95)–(2.95)) involving the coefficient matrices $Q_+(\nu)$ and $Q_-(\nu)$ is developed in Sec. 2. As it turns out, these relations can be used to construct a simple proof for the fact that the $a(4)$ scheme is neutrally stable (i.e., non-dissipative) when it is stable. Numerically, it has been established that the scheme is stable if the Courant number $|\nu| < 1/3$.

It is shown in Sec. 4 that the $a(4)$ scheme can be more accurate than the 4th-order non-dissipative $a(3)$ scheme, at least for the primary mesh variable u_j^n . However, the $a(4)$ scheme has the disadvantage that its stability bound is lower than that of the $a(3)$ scheme which is neutrally stable when $|\nu| < 1/2$.

The CESE development has been driven by a basic idea that each practical scheme be built from a non-dissipative core scheme so that the numerical dissipation can be controlled effectively. As such, development of the $a(4)$ and $a(3)$ schemes provides a foundation for the development of other more practical high order CESE schemes.

References

1. S.C. Chang and W.M. To, *A New Numerical Framework for Solving Conservation Laws—The Method of Space-Time Conservation Element and Solution Element*, NASA TM 104495, August 1991.
2. S.C. Chang, On An Origin of Numerical Diffusion: Violation of Invariance under Space-Time Inversion, in *Proceedings, 23rd Conference on Modeling and simulation, April 30-May 1, 1992, Pittsburgh, PA, USA*, edited by W.G. Vogt and M.H. Mickle, Part 5, p. 2727. Also published as NASA TM 105776.
3. S.C. Chang and W.M. To, A brief description of a new numerical framework for solving conservation laws—The method of space-time conservation element and solution element, in *Proceedings of the Thirteenth International Conference on Numerical Methods in Fluid Dynamics, Rome, Italy, 1992*, edited by M. Napolitano and F. Sabetta, Lecture Notes in Physics 414, (Springer-Verlag, New York/Berlin, 1992), p. 396.
4. S.C. Chang, X.Y. Wang, and C.Y. Chow, The method of Space-Time Conservation Element and Solution Element—Application to One-Dimensional and Two-Dimensional Time-Marching Flow Problems, AIAA Paper 95-1754-CP, appears in *A Collection of Technical Papers, Part 2, pp. 1258–1291, 12th AIAA CFD Conference, June 19-22, 1995, San Diego, California*, Also published as NASA TM 106915 (1995).
5. S.C. Chang, The method of space-time conservation element and solution Element—A new approach for solving the Navier-Stokes and Euler equations, *J. Comput. Phys.*, **119**, 295 (1995).
6. S.C. Chang, S.T. Yu, A. Himansu, X.Y. Wang, C.Y. Chow, and C.Y. Loh, The method of space-time conservation element and solution element—A new paradigm for numerical solution of conservation laws, in *Computational Fluid Dynamics Review 1998* edited by M.M. Hafez and K. Oshima (World Scientific, Singapore), Vol. 1, p. 206.
7. T. Molls and F. Molls, Space-Time Conservation Method Applied to Saint Venant Equations, *J. of Hydraulic Engr.*, **124(5)**, 501 (1998).
8. C. Zoppou and S. Roberts, Space-Time Conservation Method Applied to Saint Venant Equations: A Discussion, *J. of Hydraulic Engr.*, **125(8)**, 891 (1999).
9. S.C. Chang, X.Y. Wang, and C.Y. Chow, The space-time conservation element and solution element method: A new high-resolution and genuinely multidimensional paradigm for solving conservation laws, *J. Comput. Phys.*, **156**, 89 (1999).
10. X.Y. Wang, and S.C. Chang, A 2D non-splitting unstructured triangular mesh Euler solver based on the space-time conservation element and solution element method, *Computational Fluid Dynamics Journal*, **8(2)**, 309 (1999).
11. S.C. Chang, X.Y. Wang and W.M. To, Application of the space-time conservation element and solution element method to one-dimensional convection-diffusion problems, *J. Comput. Phys.*, **165**, 189 (2000).
12. J. Qin, S.T. Yu, Z.C. Zhang, and M.C. Lai, Direct Calculations of Cavitating Flows by the Space-Time CE/SE Method, *J. Fuels & Lubricants, SAE Transc.*, **108(4)**, 1720 (2000).
13. C.Y. Loh, L.S. Hultgren and S.C. Chang, Wave computation in compressible flow using the space-time conservation element and solution element method, *AIAA J.*, **39(5)**, 794 (2001).
14. Z.C. Zhang, S.T. Yu, and S.C. Chang, A Space-Time Conservation Element and Solution Element Method for Solving the Two- and Three-Dimensional Unsteady Euler Equations Using Quadrilateral and Hexahedral Meshes, *J. Comput. Phys.*, **175**, 168 (2002).
15. K.B.M.Q. Zaman, M.D. Dahl, T.J. Bencic, and C.Y. Loh, Investigation of A ‘Transonic Resonance’ with Convergent-Divergent Nozzles, *J. Fluid Mech.*, **463**, 313 (2002).
16. C.Y. Loh and K.B.M.Q. Zaman, Numerical Investigation of ‘Transonic Resonance’ with A Convergent-Divergent Nozzle, *AIAA J.*, **40(12)**, 2393 (2002).
17. S. Motz, A. Mitrovic, and E.-D. Gilles, Comparison of Numerical Methods for the Simulation of Dispersed Phase Systems, *Chemical Engineering Science*, **57**, 4329 (2002).
18. S. Cioc and T.G. Keith, Application of the CE/SE Method to One-Dimensional Flow in Fluid Film Bearings, *STLE Tribology Transactions*, **45**, 167 (2002).
19. S. Cioc and T.G. Keith, Application of the CE/SE Method to Two-Dimensional Flow in Fluid Film Bearings, *International J. of Numer. Methods for Heat & Fluid Flow*, **13(2)**, 216 (2003).

20. S. Cioc, F. Dimofte, T.G. Keith, and D.P. Fleming, Computation of Pressurized Gas Bearings Using the CE/SE Method, *STLE Tribology Transactions*, **46(1)**, 128 (2003).
21. S. Cioc, F. Dimofte, and T.G. Keith, Application of the CE/SE Method to Wave Journal Bearings, *STLE Tribology Transactions*, **46(2)**, 179 (2003).
22. A. Ayasoufi and T.G. Keith, Application of the Conservation Element and Solution Element Method in Numerical Modeling of Heat Conduction with Melting and/or Freezing, *International J. of Numer. Methods for Heat & Fluid Flow*, **13(4)**, 448 (2003).
23. A. Ayasoufi and T.G. Keith, Application of the Conservation Element and Solution Element Method in Numerical Modeling of Axisymmetric Heat Conduction with Melting and/or Freezing, *JSME International J. Series B*, **47(1)**, 115 (2004).
24. A. Ayasoufi and T.G. Keith, Application of the Conservation Element and Solution Element Method in Numerical Modeling of Three-dimensional Heat Conduction with Melting and/or Freezing, *Transactions of the ASME, J. of Heat Transfer*, **126(6)**, 937 (2004).
25. Y.I. Lim, S.C. Chang, and S.B. Jorgensen, A Novel Partial Differential Algebraic Equation (PDAE) Solver: Iterative Space-Time Conservation Element/Solution Element (CE/SE) Method, *Computers and Chemical Engineering*, **28**, 1309 (2004)
26. Y.I. Lim and S.B. Jorgensen, A Fast and Accurate Numerical Method for Solving Simulated Moving Bed (SMB) Chromatographic Separation Problems, *Chemical Engineering Science*, **59**, 1931 (2004).
27. Y.I. Lim, An Optimization Strategy for Nonlinear Simulated Moving Bed Chromatography: Multi-level Optimization Procedure (MLOP), *Korea J. Chem. Eng.*, **21(4)**, 836 (2004).
28. C.K. Kim, S.T. John Yu, and Z.C. Zhang, Cavity Flow in Scramjet Engine by the Space-Time Conservation Element and Solution Element Method, *AIAA J.*, **42(5)**, 912 (2004).
29. M. Zhang, S.T. John Yu, S.C. Lin, S.C. Chang, and I. Blankson, Solving Magnetohydrodynamic Equations Without Special Treatment for Divergence-Free Magnetic Field, *AIAA J.*, **42(12)**, 2605 (2004).
30. K.S. Im, M.C. Lai, S.T. John Yu, and Robert R. Matheson, Jr., Simulation of Spray Transfer Process in Electrostatic Rotary Bell Sprayer, *ASME J. of Fluid Engineering*, **126(3)**, 449 (2004).
31. S. Jerez, J.V. Romero, and M.D. Rosello, A Semi-Implicit Space-Time CE-SE Method to Improve Mass Conservation through Tapered Ducts in Internal Combustion Engines, *Math. and Computer Modeling*, **40**, 941 (2004).
32. S.C. Chang, Y. Wu, V. Yang, and X.Y. Wang, Local Time Stepping Procedures for the Space-Time Conservation Element and Solution Element Method, *International J. Comput. Fluid Dynamics*, **19(5)**, 359 (2005).
33. Y.I. Lim, S.B. Jorgensen, and I.H. Kim, Computer-Aided Model Analysis for Ionic Strength-Dependent Effective Charge of Protein in Ion-Exchange Chromatography, *Bio-Chem. Eng. J.*, **25(2)**, 125 (2005).
34. T.I. Tseng and R.J. Yang, Simulation of the Mach Reflection in Supersonic Flows by the CE/SE Method, *Shock Waves*, **14(4)**, 307 (2005).
35. B. Wang, H. He, and S.-T.J. Yu, Direct Calculation of Wave Implosion for Detonation Initiation, *AIAA J.*, **43(10)**, 2157 (2005).
36. T.I. Tseng and R.J. Yang, Numerical Simulation of Vorticity Production in Shock Diffraction, accepted for publication in *AIAA J.*
37. M. Zhang, S.-T. Yu, S.C.H. Lin, S.C. Chang, and I. Blankson, Solving the MHD Equations By the Space-Time Conservation Element and Solution Element Method, *J. Comput. Phys.*, **214**, 599 (2006).
38. S. Qamar and G. Warnecke, A Space-Time Conservation Method for Hyperbolic Systems with Stiff and Non Stiff Source Terms, *Commun. Comput. Phys.*, **1(3)**, 449 (2006).
39. X.Y. Wang, C.Y. Chow, and S.C. Chang, *Numerical Simulation of Flows Caused by Shock-Body Interaction*, AIAA Paper 96-2004 (1996).
40. C.Y. Loh, L.S. Hultgren and S.C. Chang, *Vortex Dynamics Simulation in Aeroacoustics by the Space-Time Conservation Element and Solution Element Method*, AIAA Paper 99-0359 (1999)
41. X.Y. Wang, S.C. Chang and P.C.E. Jorgenson, *Accuracy Study of the Space-Time CE/SE Method for Computational Aeroacoustics Problems Involving Shock Waves*, AIAA Paper 2000-0474 (2000).

42. C.Y. Loh, L.S. Hultgren, S.C. Chang and P.C.E. Jorgenson, *Noise Computation of a Supersonic Shock-Containing Axisymmetric Jet by the CE/SE Method*, AIAA Paper 2000-0475 (2000).
43. C.Y. Loh, X.Y. Wang, S.C. Chang, and P.C.E. Jorgenson, Computation of Feedback Aeroacoustic System by the CE/SE Method, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 555.
44. C.Y. Loh, L.S. Hultgren and P.C.E. Jorgenson, *Near Field Screech Noise Computation for An Underexpanded Supersonic Jet by the CE/SE Method*, AIAA Paper 2001-2252 (2001).
45. X.Y. Wang, S.C. Chang, and P.C.E. Jorgenson, Numerical Simulation of Aeroacoustic Field in a 2D Cascade Involving a Downstream Moving Grid Using the Space-Time CE/SE method, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 543.
46. X.Y. Wang, S.C. Chang, A. Himansu, and P.C.E. Jorgenson, *Gust Acoustic Response of A Single Airfoil Using the Space-Time CE/SE Method*, AIAA Paper 2002-0801 (2002).
47. S.T. Yu and S.C. Chang, *Treatments of Stiff Source Terms in Conservation Laws by the Method of Space-Time Conservation Element and Solution Element*, AIAA Paper 97-0435 (1997).
48. S.T. Yu and S.C. Chang, Applications of the Space-Time Conservation Element / Solution Element Method to Unsteady Chemically Reactive Flows,” AIAA Paper 97-2099, in *A Collection of Technical Papers, 13th AIAA CFD Conference*, June 29-July 2, 1997, Snowmass, CO.
49. S.T. Yu, S.C. Chang, P.C.E. Jorgenson, S.J. Park and M.C. Lai, “Treating Stiff Source Terms in Conservation Laws by the Space-Time Conservation Element and Solution Element Method,” in *Proceedings of the 16th International Conference on Numerical Method in Fluid Dynamics, Arcachon, France, 6-10 July, 1998*, edited by C.H. Bruneau, (Springer-Verlag Berlin Heidelberg 1998), p. 433.
50. X.Y. Wang and S.C. Chang, A 3D structured/unstructured Euler solver based on the space-time conservation element and solution element method, in *A Collection of Technical Papers, 14th AIAA CFD Conference, June 28–July 1, 1999, Norfolk, Virginia*, AIAA Paper 99-3278.
51. N.S. Liu and K.H. Chen, *Flux: An Alternative Flow Solver for the National Combustion Code*, AIAA Paper 99-1079.
52. G. Cook, *High Accuracy Capture of Curved Shock Front Using the Method of Conservation Element and Solution Element*, AIAA Paper 99-1008.
53. S.C. Chang, Y. Wu, X.Y. Wang, and V. Yang, Local Mesh Refinement in the Space-Time CE/SE Method, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 61.
54. S.C. Chang, Z.C. Zhang, S.T. John Yu, and P.C.E. Jorgenson, A Unified Wall Boundary Treatment for Viscous and Inviscid Flows in the CE/SE Method, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 671.
55. Z.C. Zhang, S.T. John Yu, S.C. Chang, and P.C.E. Jorgenson, Calculations of Low-Mach-Number Viscous Flows without Preconditioning by the Space-Time CE/SE method, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 127.
56. A. Himansu, P.C.E. Jorgenson, X.Y. Wang, and S.C. Chang, Parallel CE/SE Computational via Domain Decomposition, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 423.
57. Y. Wu, V. Yang, and S.C. Chang, Space-Time Method for Chemically Reacting Flows with Detailed Kinetics, in *Proceedings of the First International Conference on Computational Fluid Dynamics, Kyoto, Japan, 10-14 July, 2000*, edited by N. Satofuka, (Springer-Verlag Berlin Heidelberg 2001), p. 207.
58. I.S. Chang, *Unsteady Rocket Nozzle Flows*, AIAA Paper 2002-3884.
59. S.C. Chang, *Courant Number Insensitive CE/SE Schemes*, AIAA Paper 2002-3890 (2002).
60. I.S. Chang, *Unsteady Underexpanded Jet Flows*, AIAA Paper 2003-3885.

61. S.C. Chang and X.Y. Wang, *Multidimensional Courant Number Insensitive CE/SE Euler Solvers for Applications Involving Highly Nonuniform Meshes*, AIAA Paper 2003-5280.
62. B.S. Venkatachari, G.C. Cheng, and S.C. Chang, *Development of A Transient Viscous Flow Solver Based on Conservation Element-Solution Element Framework*, AIAA Paper 2004-3413.
63. B.S. Venkatachari, G.C. Cheng, and S.C. Chang, *Courant Number Insensitive Transient Viscous Flow Solver Based on CE/SE Framework*, AIAA Paper 2005-00931.
64. S.C. Chang, *Explicit von Neumann Stability Conditions for the c - τ Scheme—A Basic Scheme in the Development of the CE-SE Courant Number Insensitive Schemes*, NASA TM 2005-213627, April 2005.
65. J.C. Yen and D.A. Wagner, *Computational Aeroacoustics Using a Simplified Courant Number Insensitive CE/SE Method*, AIAA Paper 2005-2820.
66. I.S. Chang, C.L. Chang, and S.C. Chang, *Unsteady Navier-Stokes Rocket Nozzle Flows*, AIAA Paper 2005-4353.
67. S.C. Chang, *Courant Number and Mach Number Insensitive CE/SE Euler Solvers*, AIAA Paper 2005-4355.
68. S.C. Chang, A. Himansu, C.Y. Loh, X.Y. Wang, and S.T. Yu, *Robust and Simple Non-Reflecting Boundary Conditions for the Euler Equations—A New Approach Based on the Space-Time CE/SE Method*, in *Proceedings, NSF-CBMS Regional Research Conference on Mathematical Methods in Nonlinear Wave Propagation, North Carolina A&T State University, Greensboro, North Carolina, May 15-19, 2005*, edited by D.P. Clemence and G. Tang, p. 155-190, Vol. 379 in *Contemporary Mathematics*, American Mathematical Society (2005).
69. I.S. Chang, C.L. Chang, and S.C. Chang, *3D Unsteady Navier-Stokes Rocket Nozzle Flows*, AIAA Paper 2006-4775.
70. C.L. Chang, *Time-accurate, Unstructured-Mesh Navier-Stokes Computations with the Space-time CESE Method*, AIAA Paper 2006-4780.
71. S.C. Chang, *On Space-Time Inversion Invariance and Its Relation to Non-Dissipativeness of a CESE Core Scheme*, AIAA Paper 2006-4779.
72. S.C. Chang, *The $a(3)$ Scheme—A Fourth-Order Neutrally Stable CESE Solver*, AIAA Paper 2007-4321.
73. Other CESE references are posted on: <http://www.grc.nasa.gov/www/microbus>.
74. R.A. Horn and C.R. Johnson, *Matrix Analysis*, Cambridge University Press, 1985.

TABLE 1.—NUMERICAL RESULTS OF THE $a(4)$, $a(3)$, AND a SCHEMES

		$\nu = 0.1$		$t = 9.876$	
		$K = 25, n = 2,469$	$K = 50, n = 4,938$	$K = 100, n = 9,876$	$K = 200, n = 19,752$
E	$a(4)$	0.506×10^{-4}	0.741×10^{-6}	0.200×10^{-6}	0.348×10^{-8}
	$a(3)$	0.131×10^{-3}	0.143×10^{-4}	0.883×10^{-6}	0.549×10^{-7}
	a	0.452	0.115	0.287×10^{-1}	0.716×10^{-2}
E_x	$a(4)$	0.595×10^{-2}	0.203×10^{-2}	0.531×10^{-3}	0.132×10^{-3}
	$a(3)$	0.445×10^{-1}	0.977×10^{-3}	0.611×10^{-4}	0.382×10^{-5}
	a	2.90	0.732	0.182	0.454×10^{-1}
E_{xx}	$a(4)$	0.191	0.104×10^{-1}	0.115×10^{-1}	0.674×10^{-3}
	$a(3)$	0.225	0.169	0.406×10^{-1}	0.100×10^{-1}
E_{xxx}	$a(4)$	43.7	59.9	63.2	63.2

TABLE 2.—NUMERICAL RESULTS OF THE $a(4)$, $a(3)$, AND a SCHEMES

		$\nu = 0.1$		$t = 10.00$	
		$K = 25, n = 2,500$	$K = 50, n = 5,000$	$K = 100, n = 10,000$	$K = 200, n = 20,000$
E	$a(4)$	0.410×10^{-4}	0.152×10^{-5}	0.170×10^{-6}	0.539×10^{-8}
	$a(3)$	0.228×10^{-3}	0.110×10^{-4}	0.628×10^{-6}	0.384×10^{-7}
	a	0.469	0.118	0.292×10^{-1}	0.727×10^{-2}
E_x	$a(4)$	0.832×10^{-2}	0.161×10^{-2}	0.383×10^{-3}	0.918×10^{-4}
	$a(3)$	0.154×10^{-1}	0.992×10^{-3}	0.623×10^{-4}	0.390×10^{-5}
	a	2.89	0.728	0.182	0.455×10^{-1}
E_{xx}	$a(4)$	0.146	0.242×10^{-1}	0.978×10^{-2}	0.137×10^{-2}
	$a(3)$	0.473	0.316×10^{-1}	0.199×10^{-2}	0.124×10^{-3}
E_{xxx}	$a(4)$	61.3	47.7	45.2	43.6

TABLE 3.—NUMERICAL RESULTS OF THE $a(4)$, $a(3)$, AND a SCHEMES

		$\nu = 1/3$		$t = 9.6$	
		$K = 25, n = 720$	$K = 50, n = 1,440$	$K = 100, n = 2,880$	$K = 200, n = 5,760$
E	$a(4)$	0.569×10^{-13}	0.104×10^{-12}	0.211×10^{-12}	0.417×10^{-12}
	$a(3)$	0.190×10^{-3}	0.103×10^{-4}	0.616×10^{-6}	0.380×10^{-7}
	a	0.408	0.101	0.251×10^{-1}	0.626×10^{-2}
E_x	$a(4)$	0.844×10^{-2}	0.238×10^{-2}	0.612×10^{-3}	0.154×10^{-3}
	$a(3)$	0.947×10^{-2}	0.596×10^{-3}	0.373×10^{-4}	0.233×10^{-5}
	a	2.48	0.624	0.155	0.388×10^{-1}
E_{xx}	$a(4)$	0.151×10^{-10}	0.577×10^{-10}	0.375×10^{-9}	0.200×10^{-8}
	$a(3)$	0.672	0.129	0.294×10^{-1}	0.716×10^{-2}
E_{xxx}	$a(4)$	56.9	64.3	66.1	66.6

TABLE 4.—NUMERICAL RESULTS OF THE $a(4)$, $a(3)$, AND a SCHEMES

		$\nu = 1/3$		$t = 10.00$	
		$K = 25, n = 750$	$K = 50, n = 1,500$	$K = 100, n = 3,000$	$K = 200, n = 6,000$
E	$a(4)$	0.595×10^{-13}	0.109×10^{-12}	0.219×10^{-12}	0.435×10^{-12}
	$a(3)$	0.134×10^{-3}	0.590×10^{-5}	0.330×10^{-6}	0.200×10^{-7}
	a	0.424	0.106	0.262×10^{-1}	0.653×10^{-2}
E_x	$a(4)$	0.750×10^{-12}	0.205×10^{-11}	0.410×10^{-9}	0.198×10^{-8}
	$a(3)$	0.992×10^{-2}	0.627×10^{-3}	0.393×10^{-4}	0.246×10^{-5}
	a	2.616	0.655	0.163	0.408×10^{-1}
E_{xx}	$a(4)$	0.164×10^{-10}	0.592×10^{-10}	0.380×10^{-9}	0.203×10^{-8}
	$a(3)$	0.320	0.203×10^{-1}	0.127×10^{-2}	0.794×10^{-4}
E_{xxx}	$a(4)$	0.470×10^{-8}	0.456×10^{-7}	0.443×10^{-4}	0.857×10^{-3}

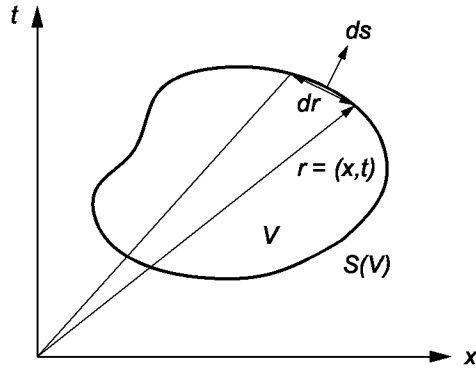
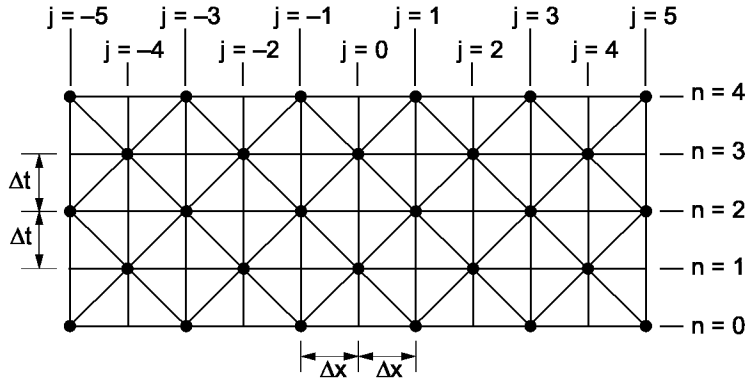
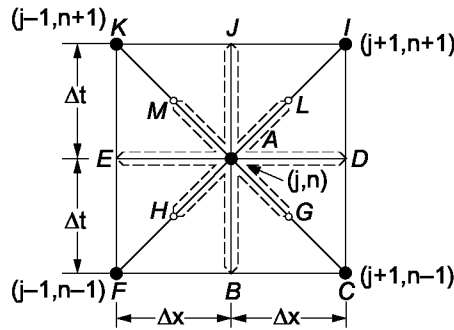


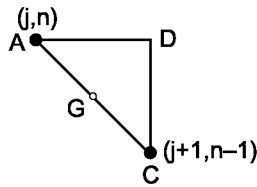
Figure 1.—A surface element on the boundary $S(V)$ of an arbitrary space-time volume V .



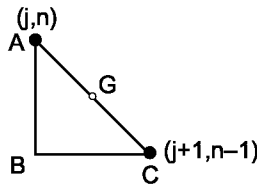
2(a).—The space-time mesh.



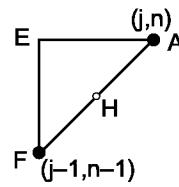
2(b).— $SE(j, n)$.



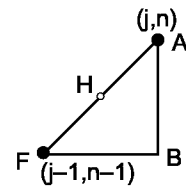
2(c).— $CE(j, n; 1)$.



2(d).— $CE(j, n; 2)$.



2(e).— $CE(j, n; 3)$.



2(f).— $CE(j, n; 4)$.

Figure 2.—The SEs and CEs.

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14. ABSTRACT The CESE development is driven by a belief that a solver should (i) enforce conservation laws in both space and time, and (ii) be built from a nondissipative (i.e., neutrally stable) core scheme so that the numerical dissipation can be controlled effectively. To provide a solid foundation for a systematic CESE development of high order schemes, in this paper we describe a new high order (4-5th order) and neutrally stable CESE solver of a 1D advection equation with a constant advection speed a . The space-time stencil of this two-level explicit scheme is formed by one point at the upper time level and two points at the lower time level. Because it is associated with four independent mesh variables (the numerical analogues of the dependent variable and its first, second, and third-order spatial derivatives) and four equations per mesh point, the new scheme is referred to as the $a(4)$ scheme. As in the case of other similar CESE neutrally stable solvers, the $a(4)$ scheme enforces conservation laws in space-time locally and globally, and it has the basic, forward marching, and backward marching forms. Except for a singular case, these forms are equivalent and satisfy a space-time inversion (STI) invariant property which is shared by the advection equation. Based on the concept of STI invariance, a set of algebraic relations is developed and used to prove the $a(4)$ scheme must be neutrally stable when it is stable. Numerically, it has been established that the scheme is stable if the value of the Courant number is less than $1/3$.					
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