ON AN ORIGIN OF NUMERICAL DIFFUSION: VIOLATION OF INVARIANCE UNDER SPACE-TIME INVERSION

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ABSTRACT

We study the invariant properties of the convection equation $\partial u/\partial t + a \partial u/\partial x = 0$ with respect to spatial reflection, time reversal, and space-time inversion. Generally, a finite-difference analogue of this equation may possess some or none of these properties. It is shown that, under certain conditions, the von Neumann amplification factor of an analogue satisfies a special relation for each invariant property this analogue possesses. Particularly, an analogue is neutrally stable and thus free of numerical diffusion if it possesses the invariant property related to space-time inversion. It is also explained why generally (*i*) an upwind scheme possesses neither the invariant property related to spatial reflection nor that related to space-time inversion, and (*ii*) an explicit scheme possesses neither the invariant property related to time reversal nor that related to spacetime inversion. Extension to the viscous case and a remarkable connection between the current work and a new numerical framework for solving conservation laws are also discussed.

1. INTRODUCTION

Many physical equations are invariant (i.e., they do not change their forms) under certain transformations. As a simple example, consider the convection equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \tag{1.1}$$

where a is an arbitrary real constant. Eq. (1.1) is equivalent to

$$\frac{\partial u}{\partial t'} + a' \frac{\partial u}{\partial x'} = 0 \tag{1.2}$$

if

x' = -x, t' = t, and a' = -a (1.3)

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(i)

(ii)
$$x' = x$$
, $t' = -t$, and $a' = -a$ (1.4)

In other words, Eq. (1.1) is mapped into the same equation under the mapping

$$x \to x', t \to t', \text{ and } a \to a'$$
 (1.5)

if x', t', and a' are defined either by Eq. (1.3) or Eq. (1.4). Since the mapping defined by Eq. (1.5) with

(iii)
$$x' = -x$$
, $t' = -t$, and $a' = a$ (1.6)

can be considered as the product of the first two mappings (in either order), Eq. (1.1) is also mapped into itself under the third mapping.

Since the mapping $(x,t) \rightarrow (x',t')$ represents (i) spatial reflection with respect to the reference plane x = 0 if x' = -x and t' = t, (ii) time reversal with respect to the reference plane t = 0 if x' = x and t' = -t, and (iii) space-time inversion with respect to the origin if x' = -x and t' = -t, Eq. (1.1) is said to possess invariant properties with respect to spatial reflection, time reversal, and space-time inversion respectively.

As a result of the above properties, solutions to Eq. (1.1) also possess similar invariant properties. Let F be a function of a real variable. Then, for any a,

$$u = u_0(x,t;a) \stackrel{\text{def}}{=} F(x-at) \tag{1.7}$$

is a solution to Eq. (1.1) if the derivative of F exists. Since (i) $u = u_0(x,t;a)$ is a solution to Eq. (1.1) if and only if $u = u_0(x',t';a')$ is a solution to Eq. (1.2), and (ii) Eq. (1.1) is equivalent to Eq. (1.2) if x', t', and a' are related to x, t and a by either Eq. (1.3) or Eq. (1.4) or Eq. (1.6), one concludes that

$$u = u_0(-x,t;-a) , \qquad (1.8)$$

$$u = u_0(x, -t; -a) , \qquad (1.9)$$

and

$$u = u_0(-x, -t; a) \tag{1.10}$$

are also solutions to Eq. (1.1) (Note: do not alter the sign of a in Eq. (1.1)). The above conclusion can also be verified directly by using the facts that $u_0(-x,t;-a) = F(-(x-at))$, $u_0(x, -t; -a) = F(x-at)$, and $u_0(-x, -t; a) = F(-(x-at))$.

Numerical schemes generally are constructed without considering the invariant properties of the physical equations to be solved [1]. As a result, numerical solutions generally do not share the same invariant properties of physical solutions. Using numerical analogues of Eq. (1.1) as examples, it will be explained in this paper how violation of the invariant property with respect to space-time inversion is related to the numerical diffusion of these analogues. Particularly, it will be shown that a two-level constant-coefficient difference analogue of Eq. (1.1) is neutrally stable and thus free of numerical diffusion if it preserves the invariant property related to space-time inversion.

The remainder of this paper is briefly described as follows: In Section 2, we investigate the invariant properties of several well known numerical analogues of Eq. (1.1). It is shown that the Wendroff scheme Eq. (2.1) and the Crank-Nicolson scheme Eq. (2.11) are invariant under (i) spatial reflection, (ii) time reversal, and (iii) space-time inversion, in a sense to be defined. Note that invariance under any two of (i) - (iii) implies invariance under the third. We also show that the invariance of a scheme under any one of (i) - (iii) cannot occur unless the configuration of its stencil satisfies a certain necessary condition. This explains why generally an upwind scheme cannot be invariant under either spatial reflection or space-time inversion while a two-level explicit scheme cannot be invariant under either time reversal or space-time inversion.

In Section 3, we consider an arbitrary two-level constant-coefficient finite-difference analogue of Eq. (1.1). It is shown that the von Neumann amplification factor of this analogue must satisfy certain relation if it is invariant under any one of the transformations referred to above. As a result, one can show that a scheme must be neutrally stable if it is invariant under space-time inversion.

In Section 4, the discussion is extended to the convection-diffusion equation Eq. (4.1). We also consider the Leapfrog/DuFort-Frankel scheme Eq. (4.22), which involves three time levels and also is invariant under all three transformations referred to above.

In Section 5, we summarize the key results obtained in the current study and explain how they can be used in a more complicated situation. We also show that, contrary to traditional two-level explicit scheme, a new two-level explicit analogue of Eq. (4.1), which is constructed by using a numerical framework currently being developed by Chang and To [2], is invariant under spatial reflection, time reversal and space-time inversion. It is also shown that there is a remarkable similarity between the forms of the amplification factors of the new scheme and the Leapfrog/DuFort-Frankel scheme. The implication of this similarity is also discussed.

2. INVARIANT PROPERTIES OF NUMERICAL SCHEMES

A two-level difference scheme which can be used to solve Eq. (1.1) is the Wendroff scheme [p.503, 3], i.e.,

$$(1+\mathbf{v})(u_{j+1}^{n+1}-u_{j}^{n}) + (1-\mathbf{v})(u_{j}^{n+1}-u_{j+1}^{n}) = 0$$
(2.1)

where

$$v \stackrel{def}{=} \frac{a\Delta t}{\Delta x} \tag{2.2}$$

is the Courant number. We assume that Eq. (2.1) is valid for $j, n = 0, \pm 1, \pm 2, \cdots$.

Given any pair of integers j_0 and n_0 , there is one equation in Eq. (2.1) with $j = j_0$ and $n = n_0$. The image of this equation under the mapping SR defined by $u_j^n \to u_{-j}^n$ $(j, n = 0, \pm 1, \pm 2, \cdots)$ and $v \to -v$ is

$$(1-\nu)\left(u_{-(j_0+1)}^{n_0+1}-u_{-j_0}^{n_0}\right)+(1+\nu)\left(u_{-j_0}^{n_0+1}-u_{-(j_0+1)}^{n_0}\right)=0$$
(2.3)

Eq. (2.3) can be rewritten as

$$(1+\nu)(u_{-(j_0+1)+1}^{n_0+1} - u_{-(j_0+1)}^{n_0}) + (1-\nu)(u_{-(j_0+1)}^{n_0+1} - u_{-(j_0+1)+1}^{n_0}) = 0$$
(2.4)

A comparison between Eq. (2.4) and (2.1) reveals that the image of the original equation is also one of Eq. (2.1) with $j = -(j_0+1)$, $n = n_0$ and the same Courant number v.

Since j_0 and n_0 are arbitrary integers, one concludes that the system of equations represented by Eq. (2.1) is mapped into itself under the mapping SR. In other words, the system of equations represented by

$$(1-\mathbf{v})(u_{-(j+1)}^{n+1}-u_{-j}^{n})+(1+\mathbf{v})(u_{-j}^{n+1}-u_{-(j+1)}^{n})=0, \quad j,n=0,\pm 1,\pm 2,\cdots$$
(2.5)

is identical to that represented by Eq. (2.1). In this paper, a scheme with this property is said to be invariant under spatial reflection.

Let R_1 be a set of real numbers such that the negative of an element is also an element. For any $v \in R_1$, let

$$u_i^n = \underline{u}_0(j,n;\mathbf{v}) , \quad j,n = 0, \pm 1, \pm 2, \cdots$$
 (2.6)

be a solution to Eq. (2.1). Since Eqs. (2.1) and (2.5) are identical, Eq. (2.6) is also a solution to Eq. (2.5), i.e.,

$$(1-v) \left[\underline{u}_{0}(-(j+1), n+1; v) - \underline{u}_{0}(-j, n; v) \right]$$

+ $(1+v) \left[\underline{u}_{0}(-j, n+1; v) - \underline{u}_{0}(-(j+1), n; v) \right] = 0$, $j, n = 0, \pm 1, \pm 2, \cdots$ (2.7)

Since Eq. (2.7) is valid for any $v \in R_1$, it is also valid if v is replaced by -v. A comparison between this new form and Eq. (2.1) reveals that, for any $v \in R_1$,

$$u_j^n = \underline{u}_0(-j,n;-v)$$
, $j,n = 0, \pm 1, \pm 2, \cdots$ (2.8)

is also a solution to Eq. (2.1). Obviously, this property is shared by any scheme which is invariant under spatial reflection. Since j is the numerical analogy of x and $v = a\Delta t/\Delta x$, this property is similar to the property that Eq. (1.8) must satisfy Eq. (1.1) if Eq. (1.7) does.

Similarly, it can be shown that the system of equations represented by Eq. (2.1) is mapped into itself under the mapping TR defined by $u_j^n \to u_j^{-n}$ $(j, n = 0, \pm 1, \pm 2, \cdots)$ and $v \to -v$. In this paper, a scheme with this property is said to be invariant under time reversal. Also it may be shown that, for any $v \in R_1$,

$$u_i^n = \underline{u}_0(j, -n; -v)$$
, $j, n = 0, \pm 1, \pm 2, \cdots$ (2.9)

must satisfy a scheme which is invariant under time reversal if Eq. (2.6) satisfies this scheme for any $v \in R_1$.

Let the mapping STI be defined by $u_j^n \to u_{-j}^{-n}$ $(j, n = 0, \pm 1, \pm 2, \cdots)$ and $v \to v$. Since any one of the three mappings SR, TR, and STI is the product of the other two mappings (in either order), the system of equations represented by Eq. (2.1) is also mapped into itself under the mapping STI. In this paper, a scheme with this property is said to be invariant under space-time inversion. Obviously, for any $v \in R_1$,

$$u_i^n = \underline{u}_0(-j, -n; \mathbf{v})$$
, $j, n = 0, \pm 1, \pm 2, \cdots$ (2.10)

must satisfy a scheme which is invariant under space-time inversion if Eq. (2.6) satisfies this scheme for any $v \in R_1$.

To proceed further, we now establish a necessary condition for a scheme to be invariant under spatial reflection. Consider the equation in Eq. (2.1) with $j = j_0$ and $n = n_0$. Its stencil S_0 is formed by the mesh points $A = (j_0, n_0)$, $B = (j_0+1, n_0)$, $C = (j_0+1, n_0+1)$, and $D = (j_0, n_0+1)$ (see Fig. 1). The image of the above equation under the mapping SR has a stencil S'_0 formed by the mesh points $A' = (-j_0, n_0)$, $B' = (-(j_0+1), n_0)$, $C' = (-(j_0+1), n_0+1)$, and $D' = (-j_0, n_0+1)$.

Since the Wendroff scheme is invariant under spatial reflection, the image referred to above is also one of Eq. (2.1) (with $j = -(j_0+1)$ and $n = n_0$). Since the configuration of the stencil of any constant-coefficient scheme (like Eq. (2.1)) does not vary as j and n take different values, one concludes that the configurations of S_0 and S'_0 must be identical. In other words, B'A'D'C' can be made to coincide with ABCD by a simple translation in the x-direction (which, of course, is true).

To further explore the significance of the above discussion, consider a constant-coefficient upwind scheme with the mesh point D missing from the stencil S_0 (and thus D' missing from S'_0). Under this circumstance, the configurations of S_0 and S'_0 are different and it is obvious that the original equation and its image cannot satisfy the same upwind scheme. As a result, the scheme cannot be invariant under spatial reflection.

Note that the spatial-reflection image of any mesh point (j,n), $j,n = 0, \pm 1, \pm 2, \cdots$, is (-j,n)(Here we assume that the plane of reflection is j = 0). Because the stencil S'_0 is formed by the spatial-reflection images of the mesh points of the stencil S_0 , S'_0 is the spatial-reflection image of S_0 . As a result of this observation, one can conclude from the above discussions that a constant-coefficient scheme cannot be invariant under spatial reflection if the configurations of its stencil and the spatial-reflection image are different.

Similarly, one can conclude that a constant-coefficient scheme cannot be invariant under time reversal (space-time inversion) if the configurations of its stencil and the time-reversal (space-time-inversion) image are different. Note that the time-reversal (space-time-inversion) image of any mesh point (j,n), $j,n = 0, \pm 1, \pm 2, \cdots$, is (j, -n) ((-j, -n)).

It has been shown that the Wendroff scheme is invariant under spatial reflection, time reversal, and space-time inversion. Another scheme which possesses the same properties is the Crank-Nicolson scheme [p.504, 3], i.e.,

$$u_{j}^{n+1} - u_{j}^{n} + \frac{v}{4} \left[u_{j+1}^{n+1} + u_{j+1}^{n} - u_{j-1}^{n+1} - u_{j-1}^{n} \right] = 0$$
(2.11)

Obviously the stencils of these two schemes satisfy the above necessary conditions for invariance under spatial reflection, time reversal, and space-time inversion.

The Lax-Wendroff scheme [p.101, 4], i.e.,

$$u_j^{n+1} = \frac{v(v+1)}{2} u_{j-1}^n + (1-v^2) u_j^n + \frac{v(v-1)}{2} u_{j+1}^n$$
(2.12)

is invariant under spatial reflection. However, its stencil does not meet the necessary condition for invariance under time reversal or space-time inversion. Generally, the stencil of an explicit upwind scheme does not meet any of the necessary conditions for invariance under spatial reflection, time reversal, and space-time inversion.

3. VON NEUMANN ANALYSIS

In this section, again we consider only the numerical analogues of Eq. (1.1). We assume that they are two-level linear difference schemes with real constant coefficients. As in Eqs. (2.1), (2.11), and (2.12), these coefficients are assumed to be functions of the Courant number v.

For any one of the schemes referred to above, let $G(v,\theta)$, $v \in R_1$, and $-\infty < \theta < +\infty$ be the amplification factor corresponding to the Fourier component $e^{ij\theta}$. Here $i \equiv \sqrt{-1}$ and θ is the phase angle variation over Δx . Then, for any $v \in R_1$ and any θ ,

$$u_{i}^{n} = [G(\mathbf{v}, \theta)]^{n} e^{ij\theta} , \quad j, n = 0, \pm 1, \pm 2, \cdots$$
(3.1)

is a solution to the scheme under consideration. Note that, given any v and θ , a two-level scheme has only one amplification factor. For any $v \in R_1$ and any θ , let

$$u_j^n = [\tilde{G}(\mathbf{v}, \theta)]^n e^{ij\theta}$$
, $j, n = 0, \pm 1, \pm 2, \cdots$ (3.2)

be another solution to the same two-level scheme. Then one must have

$$G(\mathbf{v}, \mathbf{\theta}) = G(\mathbf{v}, \mathbf{\theta}) , \quad \mathbf{v} \in R_1 , \quad -\infty < \mathbf{\theta} < +\infty$$
 (3.3)

By assumption, the coefficients of the scheme under consideration are real. It follows that the complex conjugate of a solution is also a solution. Thus Eq. (3.1) implies that, for any $v \in R_1$ and any θ ,

$$u_j^n = [\overline{G(\mathbf{v}, \theta)}]^n e^{-ij\theta} , \quad j, n = 0, \pm 1, \pm 2, \cdots$$
(3.4)

is also a solution to the same scheme. Since Eq. (3.4) will take the form of Eq. (3.2) if θ is replaced by $-\theta$, Eq. (3.3) implies that

$$\overline{G(\mathbf{v},-\mathbf{\theta})} = G(\mathbf{v},\mathbf{\theta}) , \quad \mathbf{v} \in R_1 , \quad -\infty < \mathbf{\theta} < +\infty$$
(3.5)

Let the scheme be invariant under spatial reflection, i.e., Eq. (2.8) is a solution to this scheme if Eq. (2.6) is. Then Eq. (3.1) implies that, for any $v \in R_1$ and any θ ,

$$u_j^n = [G(-v,\theta)]^n e^{-ij\theta}$$
, $j,n = 0, \pm 1, \pm 2, \cdots$ (3.6)

is also a solution to this scheme. Since Eq. (3.6) will take the form of Eq. (3.2) if θ is replaced by $-\theta$, Eq. (3.3) implies that

$$G(-\nu,-\theta) = G(\nu,\theta) , \quad \nu \in R_1 , \quad -\infty < \theta < +\infty$$
(3.7)

if the scheme is invariant under spatial reflection.

Let the scheme be invariant under time reversal, i.e., Eq. (2.9) is a solution to this scheme if Eq. (2.6) is. Then Eq. (3.1) implies that, for any $v \in R_1$ and any θ ,

$$u_j^n = [(G(-\nu, \theta))^{-1}]^n e^{ij\theta} , \quad j, n = 0, \pm 1, \pm 2, \cdots$$
(3.8)

is also a solution to this scheme. By comparing Eq. (3.8) with Eq. (3.2) and using Eq. (3.3), one concludes that

$$[G(-\nu,\theta)]^{-1} = G(\nu,\theta) , \quad \nu \in R_1 , \quad -\infty < \theta < +\infty$$
(3.9)

if the scheme is invariant under time reversal.

Similarly, it can be shown that

$$[G(\mathbf{v},-\boldsymbol{\theta})]^{-1} = G(\mathbf{v},\boldsymbol{\theta}) , \quad \mathbf{v} \in R_1 , \quad -\infty < \boldsymbol{\theta} < +\infty$$
(3.10)

if the scheme is invariant under space-time inversion.

Note that any two of Eqs. (3.7), (3.9), and (3.10) implies the third. This is a result of the fact that any one of the three mappings SR, TR, and STI is the product of the other two mappings (in either order).

By using Eqs. (3.5) and (3.10), it is easy to show that

$$\overline{G(\mathbf{v},\mathbf{\theta})} = G(\mathbf{v},-\mathbf{\theta}) = [G(\mathbf{v},\mathbf{\theta})]^{-1}$$
(3.11)

Thus we arrive at the conclusion that the scheme is neutrally stable, i.e.,

$$|G(\mathbf{v}, \theta)| = 1 , \quad \mathbf{v} \in R_1 , \quad -\infty < \theta < +\infty$$
(3.12)

if the scheme is invariant under space-time inversion.

The amplification factors of the Wendroff scheme Eq. (2.1) and the Crank-Nicolson scheme Eq. (2.11), respectively, are

$$G(\mathbf{v}, \theta) = \frac{\cos(\theta/2) - i v \sin(\theta/2)}{\cos(\theta/2) + i v \sin(\theta/2)}$$
 Wendroff (3.13)

and

$$G(\mathbf{v}, \mathbf{\theta}) = \frac{1 - \frac{i\mathbf{v}}{2}\sin\theta}{1 + \frac{i\mathbf{v}}{2}\sin\theta}$$
 Crank-Nicolson (3.14)

For the Wendroff scheme, $G(v,\theta)$ is not uniquely defined only when v = 0 and $\theta = \pm \pi$, $\pm 3\pi$, $\pm 5\pi$, \cdots . Thus we can choose R_1 to be the set of all real numbers excluding 0. For the Crank-Nicolson scheme, $G(v,\theta)$ is defined for all real v and real θ . Thus R_1 is the set of all real numbers. Since both schemes are invariant under spatial reflection, time reversal, and space-time inversion, both amplification factors satisfy Eqs. (3.5), (3.7), and (3.9) – (3.12).

Contrarily, the amplification factor

$$G(\mathbf{v}, \mathbf{\theta}) = 1 - \mathbf{v}^2 (1 - \cos \theta) - i \mathbf{v} \sin \theta \qquad -\infty < \mathbf{v}, \ \theta < +\infty \tag{3.15}$$

of the Lax-Wendroff scheme Eq. (2.12) satisfies Eqs. (3.5) and (3.7) but not any one of Eqs. (3.9) - (3.12). This is consistent with the fact that the Lax-Wendroff scheme is invariant under spatial reflection but not under either time reversal or space-time inversion.

4. EXTENSIONS

An extension to Eq. (1.1) is the convection-diffusion equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} - \mu \frac{\partial^2 u}{\partial x^2} = 0$$
(4.1)

where a and μ are arbitrary real constants. Eq. (4.1) is equivalent to

$$\frac{\partial u}{\partial t'} + a' \frac{\partial u}{\partial x'} - \mu' \frac{\partial^2 u}{\partial {x'}^2} = 0$$
(4.2)

if

(i)
$$x' = -x$$
, $t' = t$, $a' = -a$, and $\mu' = \mu$ (4.3)

or

(ii) x' = x, t' = -t, a' = -a, and $\mu' = -\mu$ (4.4)

or

(iii)
$$x' = -x$$
, $t' = -t$, $a' = a$, and $\mu' = -\mu$ (4.5)

In other words, Eq. (4.1) is mapped into itself under the mapping

$$t \to x'$$
, $t \to t'$, $a \to a'$, and $\mu \to \mu'$ (4.6)

if x', t', a', and μ' are defined by any one of (i) - (iii). Obviously, any one of the three mappings defined by Eqs. (4.6) and (4.3) - (4.5) can be considered as the product of the other two (in either order). With the same reasoning given in Section 1, Eq. (4.1) is said to possess invariant properties with respect to spatial reflection, time reversal, and space-time inversion.

Let

$$u = u_0(x,t;a,\mu)$$
 (4.7)

be a solution to Eq. (4.1). By using the above invariant properties and a argument similar to that presented in Section 1, it can be shown that

$$u = u_0(-x,t;-a,\mu)$$
(4.8)

$$u = u_0(x, -t; -a, -\mu) \tag{4.9}$$

and

$$u = u_0(-x, -t; a, -\mu) \tag{4.10}$$

are also solutions to Eq. (4.1).

Let

$$\gamma \stackrel{def}{=} \frac{2\mu\Delta t}{\left(\Delta x\right)^2} \tag{4.11}$$

Let u_j^n be the dependent variables at the mesh point (j,n) of a constant-coefficient finitedifference analogue of Eq. (4.1). Let the mappings SR', TR', and STI', respectively, be defined by $(i) u_j^n \to u_{-j}^n (j, n = 0, \pm 1, \pm 2, \cdots), v \to -v$, and $\gamma \to \gamma$, $(ii) u_j^n \to u_j^{-n} (j, n = 0, \pm 1, \pm 2, \cdots), v \to -v$, and $\gamma \to -\gamma$, and $\gamma \to -\gamma$, and $\gamma \to -\gamma$, and $(iii) u_j^n \to u_{-j}^{-n} (j, n = 0, \pm 1, \pm 2, \cdots), v \to -v$, and $\gamma \to -\gamma$. Obviously, any one of the mappings SR', TR', and STI' can be considered as the product of the other two (in either order). In this paper, an analogue of Eq. (4.1) is said to be invariant under spatial reflection (time reversal, space-time inversion) if the system of equations formed by this analogue is mapped into itself under the mapping SR' (TR', STI'). Let R_2 be a set of ordered pairs of real numbers such that both (-x, y) and (x, -y) are elements of R_2 if (x, y) is. For any $(v, \gamma) \in R_2$, let

$$u_i^n = \mu_0(j,n;v,\gamma)$$
, $j,n = 0, \pm 1, \pm 2, \cdots$ (4.12)

be a solution to a finite-difference analogue of Eq. (4.1). Then it can be shown that, for any $(v, \gamma) \in R_2$,

$$u_i^n = \underline{u}_0(-j,n;-v,\gamma)$$
, $j,n = 0, \pm 1, \pm 2, \cdots$ (4.13)

$$u_j^n = \underline{u}_0(j, -n; -\nu, -\gamma)$$
, $j, n = 0, \pm 1, \pm 2, \cdots$ (4.14)

and

$$u_i^n = \mu_0(-j, -n; v, -\gamma)$$
, $j, n = 0, \pm 1, \pm 2, \cdots$ (4.15)

respectively, are solutions to this analogue if it is invariant under spatial reflection, time reversal, and space-time inversion, respectively. Note that the proof follows a line of arguments which was used to obtain similar results in Section 2.

Also, it is obvious that the necessary conditions for invariance established in Section 2 regarding the stencil's configuration remain valid for the current extension.

Let the numerical analogue under consideration be a two-level linear difference scheme with real constant coefficients. These coefficients are assumed to be functions of v and γ . Let $G(v, \gamma, \theta)$, $(v, \gamma) \in R_2$ and $-\infty < \theta < +\infty$, be the amplification factor. Then by using a reasoning similar to that leading to Eq. (3.5), one concludes that

$$\overline{G(\mathbf{v},\mathbf{\gamma},-\mathbf{\theta})} = G(\mathbf{v},\mathbf{\gamma},\mathbf{\theta}) , \quad (\mathbf{v},\mathbf{\gamma}) \in R_2 , \quad -\infty < \mathbf{\theta} < +\infty$$
(4.16)

Similarly, by using Eqs. (4.13) - (4.15), it can be shown that (i)

$$G(-\mathbf{v},\mathbf{\gamma},-\mathbf{\theta}) = G(\mathbf{v},\mathbf{\gamma},\mathbf{\theta}) , \quad (\mathbf{v},\mathbf{\gamma}) \in R_2 , \quad -\infty < \mathbf{\theta} < +\infty$$
(4.17)

if the scheme is invariant under spatial reflection, (ii)

$$[G(-\nu,-\gamma,\theta)]^{-1} = G(\nu,\gamma,\theta) , \quad (\nu,\gamma) \in \mathbb{R}_2 , \quad -\infty < \theta < +\infty$$
(4.18)

if the scheme is invariant under time reversal, and (iii)

$$[G(\mathbf{v},-\boldsymbol{\gamma},-\boldsymbol{\theta})]^{-1} = G(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta}) , \quad (\mathbf{v},\boldsymbol{\gamma}) \in R_2 , \quad -\infty < \boldsymbol{\theta} < +\infty$$
(4.19)

if the scheme is invariant under space-time inversion. Obviously, any two of Eqs. (4.17) - (4.19) implies the third. This is a result of the fact that any one of the three mappings SR', TR', and STI' is the product of the other two mappings (in either order).

By using Eqs. (4.16) and (4.19), one has

$$\overline{G(\mathbf{v},-\boldsymbol{\gamma},\boldsymbol{\theta})} = G(\mathbf{v},-\boldsymbol{\gamma},-\boldsymbol{\theta}) = [G(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta})]^{-1}$$
(4.20)

As a result, one concludes that

$$\overline{G(\mathbf{v},-\boldsymbol{\gamma},\boldsymbol{\theta})} \cdot G(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta}) = 1 \quad , \quad (\mathbf{v},\boldsymbol{\gamma}) \in R_2 \quad , \quad -\infty < \boldsymbol{\theta} < +\infty \tag{4.21}$$

if the scheme is invariant under space-time inversion. Note that Eq. (4.21) is reduced to Eq. (3.12) when $\gamma = 0$, i.e., $\mu = 0$.

Two-level implicit schemes Eqs. (2.1) and (2.11) were given in Section 2 as examples of the numerical analogues of Eq. (1.1) which are invariant under spatial reflection, time reversal, and space-time inversion. Also we consider only two-level schemes in Section 3 and in the derivation of Eqs. (4.16) - (4.21). A three-level explicit scheme which is designed to solve Eq. (4.1) is the Leapfrog/DuFort-Frankel scheme [p.161, 4], i.e.,

$$(1+\gamma)u_j^{n+1} = (1-\gamma)u_j^{n-1} + (\nu+\gamma)u_{j-1}^n - (\nu-\gamma)u_{j+1}^n$$
(4.22)

This scheme is also invariant under spatial reflection, time reversal, and space-time inversion. It is reduced to (i) the Leapfrog scheme if $\gamma = 0$ (i.e., $\mu = 0$) and (ii) the DuFort-Frankel scheme if $\nu = 0$ (i.e., a = 0).

The amplification factors of Eq. (4.22) are

$$G_{\pm}(\mathbf{v}, \gamma, \theta) = \frac{\gamma \cos\theta - i\nu \sin\theta \pm \sqrt{(\gamma \cos\theta - i\nu \sin\theta)^2 + 1 - \gamma^2}}{1 + \gamma} , \qquad \gamma \neq -1 \qquad (4.23)$$

Since (i) $|\cos\theta| \le 1$ and $|\sin\theta| \le 1$, and (ii) $G_{\pm}(0,0,\theta) = \pm 1$, there exists a set R_2 of ordered pairs of real numbers such that (i) both (-x,y) and (x, -y) are elements of R_2 if (x,y) is, (ii) (x, -1) does not belong to R_2 for all x, and (iii)

$$\operatorname{Re}[G_+(v,\gamma,\theta)] > 0 \quad \text{and} \quad \operatorname{Re}[G_-(v,\gamma,\theta)] < 0$$

$$(4.24)$$

for all ν , γ , and θ with $(\nu, \gamma) \in R_2$ and $-\infty < \theta < +\infty$. Here $\operatorname{Re}[G_{\pm}(\nu, \gamma, \theta)]$ denotes the real part of $G_{\pm}(\nu, \gamma, \theta)$. Note that Eq. (4.24) is equivalent to

$$\operatorname{Re}[(G_{+}(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta}))^{-1}] > 0 \quad \text{and} \quad \operatorname{Re}[(G_{-}(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta}))^{-1}] < 0$$
(4.25)

Let $(v, \gamma) \in R_2$. Let

$$u_j^n = [\tilde{G}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta})]^n e^{ij\boldsymbol{\theta}}$$
(4.26)

be a solution to Eq. (4.22). As a result of Eq. (4.24), one has

$$\tilde{G}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta}) = \begin{cases} G_{+}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta}) & \text{if } \operatorname{Re}[\tilde{G}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta})] > 0 \\ G_{-}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta}) & \text{if } \operatorname{Re}[\tilde{G}(\mathbf{v}, \boldsymbol{\gamma}, \boldsymbol{\theta})] < 0 \end{cases}$$
(4.27)

With the aid of Eqs. (4.24) - (4.27) and the fact that Eq. (4.22) is invariant under spatial reflection, time reversal, and space-time inversion, a line of arguments which were used to obtain Eqs. (3.5), (3.7), (3.9), (3.10), and (3.11) again can be invoked to show that

$$G_{\pm}(\mathbf{v},\mathbf{y},-\mathbf{\theta}) = G_{\pm}(\mathbf{v},\mathbf{y},\mathbf{\theta})$$
(4.28)

$$G_{\pm}(-\nu,\gamma,-\theta) = G_{\pm}(\nu,\gamma,\theta) \tag{4.29}$$

$$[G_{\pm}(-\nu,-\gamma,\theta)]^{-1} = G_{\pm}(\nu,\gamma,\theta)$$
(4.30)

$$[G_{\pm}(\mathbf{v},-\boldsymbol{\gamma},-\boldsymbol{\theta})]^{-1} = G_{\pm}(\mathbf{v},\boldsymbol{\gamma},\boldsymbol{\theta}) \tag{4.31}$$

and

$$G_{\pm}(\mathbf{v},-\gamma,\theta) \cdot G_{\pm}(\mathbf{v},\gamma,\theta) = 1$$
(4.32)

for all v, γ , and θ with $(v, \gamma) \in R_2$ and $-\infty < \theta < +\infty$.

Note that

$$G_{\pm}(\mathbf{v},0,\theta) = -i\mathbf{v}\sin\theta \pm \sqrt{1 - \mathbf{v}^2\sin^2\theta}$$
(4.33)

Thus $|G_{\pm}(v,0,\theta)|=1$ if $|v| \le 1$. This result is consistent with Eq. (4.32).

5. DISCUSSION AND CONCLUSION

In this paper we study several invariant properties of the numerical analogues of Eq. (1.1). Particularly, it is shown that an arbitrary two-level constant-coefficient finite-difference analogue of Eq. (1.1) is neutrally stable if it is invariant under space-time inversion. A similar study for Eq. (4.1) is also presented.

Since it is a common experience that the local behaviors of a nonlinear variable-mesh scheme may be predicted by using a local analysis (such as the von Neumann analysis) in which the dynamic coefficients and geometric parameters are frozen at their local values, the information gained and the techniques developed in the current study may also be useful in a similar study for a numerical analogue of nonlinear physical equations.

As noted previously, the construction of a numerical scheme generally does not take into account the invariant properties of the physical equations to be solved. For an upwind scheme, the stencil contains more mesh points on the upwind side than on the downwind side. Thus the configuration of the stencil differs from those of its spatial-reflection image and space-timeinversion image. According to a discussion given in Section 2, this implies that the scheme is not invariant under either spatial reflection or space-time inversion. The stronger the upwind bias is, the further away this scheme tends to be from preserving these two invariances. According to analysis presented in Section 3, this also tends to increase numerical diffusion.

For a two-level explicit scheme, the stencil generally contains several mesh points at the lower time level while only one at the upper time level. Thus the configuration of the stencil differs from those of its time-reversal image and space-time-inversion image. This implies that the scheme is not invariant under either time reversal or space-time inversion. Generally, the higher the order of accuracy of a scheme is, the more points will be at the lower time level of the stencil. In turn, this makes the scheme further away from preserving these two invariances.

Currently, a new numerical framework for solving conservation laws — the method of spacetime conservation element and solution element is being developed by Chang and To [2]. This framework is fundamentally different from the well established methods, i.e., finite difference, finite volume, finite element, and spectral methods, in both concept and methodology. It may be used to solve both inviscid and viscous flow problems.

A two-level explicit numerical analogue of Eq. (4.1) was constructed using this framework [2]. An unique feature of this scheme is that there are two dependent variables and two equations associated with each solution element. These two variables may be considered as the numerical analogues of u and $\partial u/\partial x$. Because of this feature, contrary to traditional two-level explicit schemes, it is invariant under spatial reflection, time reversal, and space-time inversion (to be shown in another paper). Its two amplification factors are $[\sigma_{\pm}(v, \hat{\gamma}, \theta)]^2$ with

$$\sigma_{\pm}(\mathbf{v},\hat{\gamma},\theta) \stackrel{\text{def}}{=} \frac{\hat{\gamma}\cos(\frac{\theta}{2}) - i\,\mathbf{v}\sin(\frac{\theta}{2}) \pm \sqrt{\left[\hat{\gamma}\cos(\frac{\theta}{2}) - i\,\mathbf{v}\sin(\frac{\theta}{2})\right]^2 + 1 - \hat{\gamma}^2}}{1 + \hat{\gamma}} \tag{5.1}$$

where $\hat{\gamma} \stackrel{\text{def}}{=} 2\gamma/(1-\nu^2)$ and $1-\nu^2 > 0$ [2]. A comparison between Eqs. (5.1) and (4.23) reveals that the expression on the right side of Eq. (4.23) can be converted to that on the right side of Eq. (5.1) if γ , ν , and θ , respectively, are replaced by $\hat{\gamma}$, ν , and $\theta/2$. Because of this remarkable similarity, it can be shown [2] that the stability condition of the new scheme, as in the case of the Leapfrog/DuFort-Frankel scheme, is essentially the CFL condition and thus independent of the viscosity coefficient μ . Therefore, the new scheme is unconditionally stable in the case of pure diffusion. Also, as in the case of the Leapfrog/DuFort-Frankel scheme, the new scheme has no numerical diffusion in the absence of viscosity.

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