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Group Velocity Interpretation of the Stability Theory of Gustafsson, Kreiss, and Sundström

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The existing stability theory for finite difference models of hyperbolic initial boundary value problems, due to Gustafsson, Kreiss, and Sundström, is difficult to understand in its original algebraic formulation. Here it is shown that the GKS stability criterion has a physical interpretation in terms of group velocity: if the finite difference model together with its boundary conditions can support a set of waves at the boundary with group velocities pointing into the field, then it is unstable. This interpretation is valid for both dissipative and nondissipative difference models. A simple argument explains why such a set of waves is unstable, and yields a new theorem on what kind of unstable growth to expect. Examples are given in one and two space dimensions.

0. INTRODUCTION

When time-dependent partial differential equations are solved numerically by finite-difference methods, more boundary conditions are usually required than the physics of the problem provides. This necessitates a selection of additional numerical boundary conditions, and in this choice an overriding consideration is numerical stability. For the case of hyperbolic equations, the stability question is solved in principle by the theory of Gustafsson, Kreiss, and Sundström [10]—henceforth "GKS." (Important contributions to this problem were also made by S. Osher.) Application of this theory, however, has been hindered by its complexity and abstractness. The purpose of this paper is to point out that the main result of the GKS theory has a simple physical interpretation in terms of *group velocity*. This interpretation does not provide an alternative to the algebraic stability test of the GKS theory, which may in practice be difficult to carry out, but it makes the meaning of the algebra clear. It also leads to a proof that except for certain borderline cases, GKS-unstable models are unstable not only in the complicated norm of [10], but in the l_2 norm also.

Group velocity is a concept associated with energy propagation under dispersive

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equations, not hyperbolic ones. Its significance to numerical stability results from the fact that finite difference models, even of nondispersive equations, are necessarily dispersive. A general discussion of group velocity effects in finite difference models can be found in [14]. For this one should also see the work of R. Vichnevetsky, which has recently been collected in [17]. The particular topic of the present paper is treated in greater detail in [15], and a rigorous development of these and various related results will be given in [16].

In the first section we look at a simple example to illustrate the group velocity idea. Section 2 extends this to the general setting of GKS. Section 3 applies these results to define certain general classes of unstable difference models, in several space dimensions as well as one, which generalize examples that have appeared in the literature.

1. An Example

Consider the model problem

$$u_t = u_x \tag{1.1}$$

for $x \in (-\infty, \infty)$, $t \in [0, \infty)$, with initial conditions

$$u(x, 0) = f(x). \tag{1.2}$$

Such an initial-value problem on a domain without boundary is called a *Cauchy problem.* The exact solution is $u(x, t) = f(x + t)$, a leftward translation at speed 1. In a Fourier or normal mode analysis of (1.1), one looks for wave solutions

$$u(x, t) = e^{i(\omega t - \xi x)}, \tag{1.3}$$

where ω is the (temporal) *frequency* and ξ is the *wavenumber*. Equation (1.1) implies that ω and ξ are related by

$$\omega = -\xi, \tag{1.4}$$

which is called the *dispersion relation* for (1.1).

Let us set up a uniform grid with space step h and time step k, and approximate $u(x, t)$ by a grid function v_j^n:

$$v_j^n \approx u(jh, nk), \qquad -\infty < j < \infty, \quad n \geqslant 0.$$

One of the simplest difference models for (1.1) is the *leapfrog* (LF) formula

$$v_j^{n+1} = v_j^{n-1} + \lambda(v_{j+1}^n - v_{j-1}^n), \tag{1.5}$$

where λ is the *mesh ratio* or Courant number k/h. We assume throughout that although h and k may decrease to 0, λ remains fixed. For $\lambda < 1$ the leapfrog scheme is stable; we say that LF is *Cauchy stable*. By substituting (1.3) into (1.5), one obtains the dispersion relation for LF,

$$e^{i\omega k} = e^{-i\omega k} + \lambda[e^{-i\xi h} - e^{i\xi h}],$$

that is,

$$\sin \omega k = -\lambda \sin \xi h. \tag{1.6}$$

This relation approximates (1.4) only for small ωk and ξh—that is, only for waves that are well resolved on the grid.

Since ω is no longer a linear function of ξ, the LF model is said to be *dispersive*. Assume for the moment that ξ and ω are real. According to a theory going back to Lord Rayleigh [4, 5, 12, 18], energy associated with wave number ξ will propagate at a *group velocity* given by

$$C = \frac{d\omega}{d\xi}. \tag{1.7}$$

(The group velocity is not the same as the phase velocity, $c = \omega/\xi$. Readers unfamiliar with this distinction are encouraged to read the discussions in [5, 12, 18].) For LF one obtains, by differentiating (1.6) implicitly,

$$C = -\cos \xi h / \cos \omega k. \tag{1.8}$$

It is apparent that energy associated with different wavenumbers or frequencies will travel at different group velocities, so that an initial signal that is not monochromatic will change form as it propagates. For a well resolved wave one has $\xi h \approx 0$ and $\omega k \approx 0$, hence $\omega k \approx -\lambda \xi h$ by (1.6), and (1.8) becomes

$$C = -1 + \tfrac{1}{2}(1 - \lambda^2)(\xi h)^2 + O((\xi h)^4). \tag{1.9}$$

Thus typical signals travel leftward at a speed less than the ideal speed 1, with higher wavenumbers lagging more than lower ones. This dispersion of wavenumbers gives rise to the spurious oscillations near discontinuities that are familiar in finite difference computations. Alternatively, if one sets up a wave packet consisting of energy at essentially constant ω and ξ, the packet will be seen to move leftward with little change of shape at the velocity (1.8) $\approx$ (1.9). For illustrations see [14, 17].

The key to our analysis is that (1.8) is valid not only for well-resolved waves, but for all waves supportable on the grid that have real wavenumber and frequency. In fact for many waves, C has the wrong sign, so that energy travels *in the wrong direction*. In particular, (1.8) gives the following group velocities for four extreme situations—the constant function and three *parasitic waves* that are sawtoothed in x

and/or t. Note that because of "aliasing" due to the discreteness of the grid, it is enough to consider values of ξh and ωk in the range $[-\pi, \pi]$.

(a) $(\xi h, \omega k) = (0, 0)$ $\quad C = -1$,

(b) $(\xi h, \omega k) = (\pi, 0)$ $\quad C = 1$,

(c) $(\xi h, \omega k) = (0, \pi)$ $\quad C = 1$,

(d) $(\xi h, \omega k) = (\pi, \pi)$ $\quad C = -1$.

Line (b) implies, for example, that if initial data are supplied to LF of the form

$$\begin{aligned} v_j^0 = v_j^1 &= (-1)^j \qquad (jh \leqslant \varepsilon), \\ &= 0 \qquad (jh > \varepsilon), \end{aligned} \tag{1.10}$$

for some $\varepsilon \gg h > 0$, then the result as t increases will approximate a steady rightward motion of the wavefront from $x = \varepsilon$ at speed 1. See [14, Fig. 6].

Now let us turn to an initial boundary value problem. Let (1.1) and (1.2) be given on the quarter plane $x, t \geqslant 0$; no boundary data at $x = 0$ are needed to make this problem well posed. To obtain an approximate solution on the grid $j, n \geqslant 0$, we can specify initial values v_j^0 and v_j^1 for $j \geqslant 0$, and apply LF for $n \geqslant 2$ at points $j \geqslant 1$. An additional boundary formula is then needed for v_0^n, $n \geqslant 2$.

Suppose we (foolishly) pick the boundary formula

$$v_0^{n+1} = \tfrac{1}{2}(v_0^n + v_2^n) \qquad (n \geqslant 1) \tag{1.11}$$

and proceed to step forward in time. Now imagine that at some time step a perturbation (e.g., rounding or truncation error) happens to be introduced that has form (1.10). It is easy to see that such a wave satisfies (1.11), and therefore this mode will behave very nearly as if the domain were still $(-\infty, \infty)$: the wave front will begin to propagate rightwards into $x \geqslant 0$ at speed 1. The initial perturbation, with sum-of-squares energy on the order of ε, will give rise to a growing solution with energy on the order of $\varepsilon + t$. Since ε might be arbitrarily small, this amounts to an amplification of the initial perturbation by an unbounded factor. *The difference scheme is unstable because there exists a rightgoing wave that satisfies both the interior formula* (1.5) *and the boundary condition* (1.11). By "rightgoing" we mean having positive group velocity.

One can verify experimentally that scheme (1.5), (1.11) is susceptible to an unstable rightgoing mode of type (b). Figure 1 shows a computation on a grid with $h = \frac{1}{40}$, $\lambda = \frac{1}{2}$. For initial data we took $v_j^0 = v_j^1 = 0$ for all j except for the arbitrary nonzero initial values

$$v_1^0 = 1, \qquad v_0^1 = \tfrac{1}{2}, \qquad v_1^1 = \tfrac{1}{3}. \tag{1.12}$$

Figures 1a–1c show the resulting solution at steps $n = 1, 4, 40$, i.e., $t = 0.0125$, 0.05, 0.5. Obviously, the expected mode has been excited, and apparently no others. In a realistic computation, truncation errors would cause a similar radiation of energy in

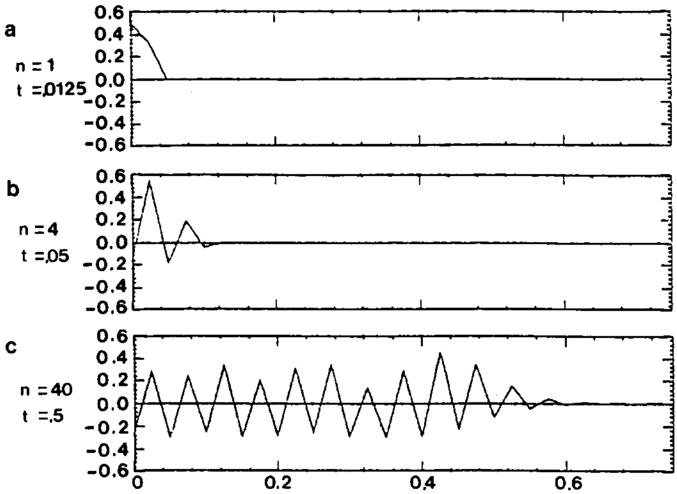

FIG. 1. Appearance of an unstable rightgoing parasitic wave in the leapfrog model (1.5), (1.11) with initial conditions (1.12).

this mode from the boundary. From (1.8) one can see that there are many other rightgoing modes for LF—in fact, any wave with $\xi h < \pi/2$ and $\omega k > \pi/2$ or $\xi h > \pi/2$ and $\omega k < \pi/2$. Mode (c) is the simplest example. None of these lead to instabilities, however, because none of them satisfy (1.11).

The main GKS theorem asserts, roughly, that an initial boundary value problem model is stable if and only if

(i) the interior difference formula is Cauchy stable,

(ii) the model (including boundary conditions) admits no eigensolutions that grow from each time step to the next by a constant factor z with $|z| > 1$, and

(iii) the model (including boundary conditions) admits no wave solutions with group velocity $C \geqslant 0$.

In practice, (i) is easy to verify, and there are rarely any growing modes of type (ii). The critical condition is therefore (iii). We shall state the GKS theory more precisely in the next section.

To obtain stability in the present example, we might replace (1.11) by the condition

$$v_0^{n+1} = \tfrac{1}{2}(v_0^n + v_1^n). \tag{1.13}$$

Then it is not hard to verify that (ii) is satisfied, and the only wavelike mode admitted by the difference model is $(\xi h, \omega k) = (0, 0)$, which has $C = -1 < 0$, hence cannot cause radiation from the boundary. Thus (iii) is satisfied and the model is stable.

It may seem that the kind of energy growth in Fig. 1 is too weak to be dangerous, and should not be considered unstable. Even mild growth of this kind, however, will in general prevent convergence as the mesh is refined. In addition, the rightgoing radiation we have described may in various circumstances lead to more catastrophic unstable growth. For one example, when a rightgoing signal of constant amplitude can occur, then sometimes similar signals with amplitudes growing linearly with n or faster are also possible. Such noise might soon become significant even though it began at the level of rounding error. Second, if the semiinfinite region $x \geqslant 0$ is replaced by a bounded strip such as $[0, 1]$, then a wavelike instability of type (iii) may be converted by repeated reflections back and forth to an exponential growth of type (ii), which is unambiguously unstable. Third, the rate of growth may also be increased if variable coefficients or lower order (undifferentiated) terms are present. The GKS theory shows that by ruling out the relatively weak instability of Fig. 1, one can be certain that these more serious effects are also excluded.

In summary, GKS instability amounts to the spontaneous radiation of energy from the boundary into the interior. In a realistic physical application, this is likely to cause trouble.

2. General Statement of the GKS Theory

Consider now a first-order hyperbolic system

$$\frac{\partial}{\partial t} u(x, t) = A \frac{\partial}{\partial x} u(x, t), \tag{2.1}$$

where u is an N-vector and A is a constant nonsingular diagonalizable matrix of dimension $N \times N$. (All of what follows extends to equations that include a zeroth-order term $Bu(x, t)$ and a forcing function $F(x, t)$.) Let (2.1) be modeled in $x \geqslant 0$ by a fixed $(s + 2)$-level Cauchy stable difference formula, explicit or implicit, dissipative or nondissipative, whose stencil extends l points to the left and r points to the right of center. For example, LF has $s = 1$ and $l = r = 1$. We can write the difference model formally as

$$Q_{-1} v^{n+1} = \sum_{\sigma=0}^{s} Q_\sigma v^{n-\sigma}, \tag{2.2}$$

where $v_j^n \approx u(jh, nk)$ is an N-vector for each j and n, and each Q_σ is a difference operator with matrix coefficients of size $N \times N$. For simplicity we assume that each Q_σ is constant, independent of h, and we assume further that the matrices Q_σ are simultaneously diagonalizable.

If (2.2) is applied for $j \geqslant l$, then boundary formulas are required to determine values v_j^n for $j = 0,..., l-1$. These can be written in the form

$$v_j^{n+1} = S_j(\{v_i^{n-\nu}\}_{0 \leqslant i \leqslant \mu}, ..., \{v_i^n\}_{0 \leqslant i \leqslant \mu}, \{v_i^{n+1}\}_{l \leqslant i \leqslant \mu}), \qquad 0 \leqslant j \leqslant l-1, \tag{2.3}$$

where μ and ν are some integers and each S_j is a linear function of its arguments.

These formulas comprise both physical boundary conditions, such as couplings between outflowing and inflowing components of v, and additional purely numerical boundary conditions. Unfortunately, it would take many pages to state precisely the form of the difference model and the assumptions it must satisfy, so for details the reader is referred to [10, sects. 1 and 5] and to [7, sect. 4], where the presentation is clearer.

The GKS theory is based on a *normal mode analysis* of what solutions model (2.2), (2.3) can support. To find the normal modes, let us begin by ignoring the boundary conditions (2.3). In the last section we looked for wavelike solutions (1.3) with frequency ω and wavenumber ξ. Let us now write

$$z = e^{i\omega k}, \qquad \kappa = e^{-i\xi h}. \tag{2.4}$$

If ω or ξ is real, then $|z| = 1$ or $|\kappa| = 1$, respectively, but we permit ω and ξ to be complex. The vector analog of (1.3) then takes the form

$$v_j^n = z^n \kappa^j \psi, \tag{2.5}$$

where ψ is a constant nonzero N-vector. Now suppose that instead of taking $|z| = 1$, we let z be any complex number with $|z| > 1$. Then there are still modes of the form (2.5), but now κ will become complex also, with $|\kappa| \neq 1$. (The circumstance $|z| > 1$, $|\kappa| = 1$ would violate the von Neumann condition, and we have assumed that (2.2) in Cauchy stable.) Figure 2 suggests the two possibilities $|\kappa| < 1$ and $|\kappa| > 1$. From one time step to the next, each mode in Fig. 2 increases in amplitude by a ratio $|z|$. It is obvious, however, that we may view this equivalently as a lateral motion, rightward in case (a) and leftward in case (b), combined with a change of phase. We will call these *rightgoing* and *leftgoing* modes, respectively.

Modes of form (2.5) do not always span the set of solutions with time dependence z^n. If several κ's coalesce for some z, then a defective situation may result in which a p-parameter collection of modes with the same ψ is permitted for some $p > 1$,

$$v_j^n = z^n \kappa^j j^\delta \psi \qquad (0 \leqslant \delta \leqslant p-1). \tag{2.6}$$

(The defective situation $p > 1$ is rarely important in practice.) A fundamental lemma of [10] now states

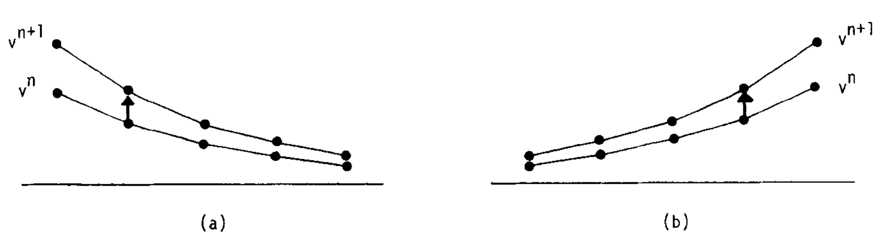

FIG. 2. Sketch of signals $v_j^n = \kappa^j z^n$ with $|z| > 1$. (a) Rightgoing, $|\kappa| < 1$. (b) Leftgoing, $|\kappa| > 1$.

PROPOSITION ([10, Lemma 5.2]). *For any z with* $|z| > 1$, (2.2) *admits a total of exactly Nl linearly independent solutions of type* (2.6) *with* $|\kappa| < 1$, *and exactly Nr such solutions with* $|\kappa| > 1$. ∎

This result is proved by reducing the difference model to a recurrence relation in j. From it we get the general solution to (2.2) that varies with z^n. Let $\{\kappa_i, \delta_i, \psi_i\}$ for $1 \leqslant i \leqslant N(l+r)$ be an enumeration of the parameters defining the solutions above, with $|\kappa_i| < 1$ for $i \leqslant Nl$ and $|\kappa_r| > 1$ otherwise.

PROPOSITION. *For any z with* $|z| > 1$, *the general solution to* (2.2) *of the form* $v_j^n = z^n \phi_j$ *can be written*

$$v_j^n = z^n \sum_{i=1}^{Nl} a_i \kappa_i^j j^{\delta_i} \psi_i + z^n \sum_{i=Nl+1}^{Nl+Nr} a_i \kappa_i^j j^{\delta_i} \psi_i \tag{2.7}$$

for arbitrary constants a_i. ∎

We may think of (2.7) as describing a linear combination of *Nl* rightgoing and *Nr* leftgoing modes.

Now let us reintroduce the boundary conditions. The full model can support only any solutions (2.7) that satisfy (2.3) as well as (2.2). There are *Nl* boundary formulas, and (2.7) depends on $N(l+r)$ free parameters, so one may expect that there will normally be an *Nr*-dimensional space of solutions that the model supports. In such a solution, a combination of leftgoing waves hits the boundary and reflects as a combination of rightgoing waves. This kind of configuaration is in general not unstable, even though the reflected energy may be larger than the incident energy. But occasionally it may happen that some collection of rightgoing signals satisfies (2.2) and (2.3) by itself, i.e., without any stimulation by leftgoing signals. In this case the left–right reflection coefficient has often become infinite. Then the model has an instability of the *Godunov–Ryabenkii* (G–R) type [13].

GODUNOV–RYABENKII THEOREM. *Suppose that for some z with* $|z| > 1$, *model* (2.2), (2.3) *admits a nonzero solution of the form*

$$v_j^n = z^n \phi_j = z^n \sum_{i=1}^{Nl} a_i \kappa_i^j j^{\delta_i} \psi_i, \tag{2.8}$$

where, as in (2.7), *each* κ_i *satisfies* $|\kappa_i| < 1$. *Then it is unstable.*

Proof. If $v_j^\sigma = z^\sigma \phi_j$ is taken as initial data for $0 \leqslant \sigma \leqslant s$, the solution as n increases will be $v_j^n = z^n \varphi_j$ for all n. Since $t = nk$, this means that v will grow like $|z|^{t/k}$. With $|z| > 1$ this growth is unbounded for any t as $k \to 0$. ∎

A similar solution made up of leftgoing waves would of course also grow unboundedly in amplitude, but this would amount to propagation of energy leftward from infinity rather than generation of energy at the boundary. The initial wave would not have finite size in l_2 or any other reasonable norm, and could not be excited by rounding errors or other perturbations. The wave ϕ in (2.8), on the other hand, does belong to l_2, and is called an *eigensolution* of the difference model.

The set of potential eigensolutions ϕ, since they are made up of rightgoing signals only, is spanned by Nl free parameters, which exactly matches the number of boundary conditions (2.3). Therefore the G–R condition has this algebraic form: does there exist, for any $|z| > 1$, a nontrivial solution of a certain system of Nl linear homogeneous equations in Nl unknowns that depends on z? Hence the problem can be cast as a *determinant condition* involving an $Nl \times Nl$ matrix $M(z)$. (For examples see [6, 7, 10].)

GODUNOV–RYABENKII THEOREM (determinant condition). *A necessary condition for stability of model* (2.2), (2.3) *is*

$$\det M(z) \neq 0 \tag{2.9}$$

for all z with $|z| > 1$.

A virtue of normal mode analysis is that in principle the determinant condition can be verified mechanically, although in practice this may be very difficult [7]. In contrast, stability proofs by the energy method [11, 13] require a measure of intuition and luck.

The limitation of the G–R condition is that although it is a necessary condition for stability, it is far from sufficient. To obtain a condition that is sufficient or nearly so, one must investigate the borderline case $|z| = 1$. This is the main achievement of the GKS theory. From the GKS point of view, this investigation is a matter of showing algebraically that certain resolvent estimates obtained for $|z| > 1$ extend continuously to $|z| = 1$. From our point of view, it is a matter of observing that the ideas of "leftgoing" and "rightgoing" still make sense as $|z| \to 1$, because in the limit $|z| = 1$ the lateral motion in Fig. 2 becomes a group velocity.

First we examine the GKS approach. For $|z| = 1$, what unstable solutions along the lines of (2.7), but also including components with $|\kappa| = 1$, can (2.2), (2.3) support? The GKS theory gives the following answer based on a *perturbation test*: First, one can rule out components with $|\kappa| > 1$, as before. One then investigates: are there any nonzero solutions to (2.2) and (2.3) of the form

$$v_j^n = z^n \phi_j = z^n \sum_i a_i \kappa_i^j j^{\delta_i} \psi_i \tag{2.10}$$

with $|\kappa_i| \leqslant 1$ for each i, for some z with $|z| \geqslant 1$? If not, the model is stable. If so, a further test is required. Given a solution (2.10), let z be perturbed slightly to a new value $\tilde{z}$ with $|\tilde{z}| > 1$. Each κ_i with $|\kappa_i| = 1$ will then move to a nearby value $\tilde{\kappa}_i$ with $|\tilde{\kappa}_i| \neq 1$. If every κ_i for which $a_i \neq 0$ in (2.10) moves to $|\tilde{\kappa}_i| < 1$, then (2.10) is an unstable mode and the model is unstable. A solution ϕ of this sort with $|z| = 1$ and $|\kappa_i| = 1$ for at least one κ_i is called a *generalized eigensolution* of the difference model. The qualification "generalized" has been introduced because such a solution no longer belongs to l_2.

The GKS stability theorem can now be stated.

GKS STABILITY THEOREM. *Model* (2.2), (2.3) *is stable if and only if* (2.2) *and* (2.3) *admit no eigensolutions or generalized eigensolutions with* $|z| \geqslant 1$.

A simpler but less constructive way to express the same theorem is by means of the determinant condition. It turns out that the $Nl \times Nl$ matrix $M(z)$, which for $|z| > 1$ embodies the condition that there be an eigensolution of G–R type, has a continuous extension to $|z| = 1$. Let $M(z)$ for $|z| \geqslant 1$ denote this extension. Then one has the

GKS STABILITY THEOREM (determinant condition). *A necessary and sufficient condition for stability of the model* (2.2), (2.3) *is*

$$\det M(z) \neq 0$$

for all z *with* $|z| \geqslant 1$.

Proof. This result is stated in [9], as Lemma 10.3 and the sentence following. ∎

Now we examine the group velocity interpretation. Suppose that (2.2) admits a solution $z^n \kappa^j$ (2.5) with $|\kappa| = |z| = 1$. Then it can be shown [15, 16] that the Cauchy stability of (2.2) implies that for values $\tilde{\kappa}$ in a neighborhood of κ, (2.5) determines a unique number $\tilde{z}(\tilde{\kappa})$ such that $v_j^n = \tilde{z}^n \tilde{\kappa}^j$ is also a solution, with $\tilde{z} \to z$ as $\tilde{\kappa} \to \kappa$. Moreover, this function $\tilde{z}(\tilde{\kappa})$ is analytic at κ, so in particular the derivative $d\tilde{z}/d\tilde{\kappa}|$

It can further be shown, again on the assumption of Cauchy stability, that C must be real, and that it governs the rate of energy flow for the solution κ, z as we have described. *Thus every solution with* $|z| = |\kappa| = 1$ *has a well-defined group velocity.*

The above conclusions hold even for dissipative difference schemes, for which $\tilde{\omega}(\tilde{\xi})$ will in general be complex when $\tilde{\xi}$ is real. What distinguishes dissipative difference schemes is only that they cannot admit solutions with $|z| = |\kappa| = 1$ except with $\kappa = 1$, so that there are fewer potentially unstable rightgoing modes to worry about. See [15, Sect. 4.4] for a discussion of stability for dissipative models.

Now if $C > 0$, then (2.11) implies that $d\tilde{z}/z$ and $d\tilde{\kappa}/\kappa$ have equal and opposite signs at $(\tilde{\kappa}, \tilde{z}) = (\kappa, z)$. In other words, κ moves inside the unit circle when z moves outside. Conversely, if $C < 0$, κ moves outside the circle when z does, and solution (2.10) does not represent a generalized eigensolution. Thus *the* GKS *perturbation test for generalized eigensolutions corresponds to a test for positive group velocities*. To determine whether a difference model is stable it is still necessary to find all solutions (2.10) and test them for instability, but viewing this test as a group velocity calculation makes the physical meaning of this procedure apparent. Moreover, since it is usually easy to compute a general formula for group velocity as a function of ξ and ω, at least for nondissipative models, the group velocity analysis often simplifies the algebra, too.

The argument of the example in Section 1 explains why a solution made of waves with positive group velocities should be unstable. The same idea leads naturally to the following necessary condition for stability in the general case:

THEOREM 1. *Suppose that model* (2.2), (2.3) *admits a solution of form* (2.10) *with* $|z|=1$, *where for each* κ_i *with* $|\kappa_i|=1$, $\delta_i=0$ *and the group speed defined by* (2.11) *satisfies* $C_i \geqslant 0$. *Suppose that for at least one such* κ_i, *say* κ_I, $C_I > 0$. *Then the model is unstable.*

In fact, we can be more precise.

THEOREM 2. *Suppose that model* (2.2), (2.3) *admits an unstable generalized eigensolution as described in Theorem* 1. *Then there exists a constant* $\rho > 0$ *such that if* $\varepsilon > 0$ *and* $t \geqslant 0$ *are arbitrary, then for all sufficiently small* h, k, *there exists a set of initial data* $\{v^\sigma\}$, $0 \leqslant \sigma \leqslant s$, *such that*

$$|v_j^\sigma| \leqslant 1 \quad \text{for} \quad j \geqslant 0, \quad 0 \leqslant \sigma \leqslant s,$$
$$v_j^\sigma = 0 \quad \text{for} \quad jh > \varepsilon, \quad 0 \leqslant \sigma \leqslant s,$$

and

$$\| v^{t/k} \|_2^2 \geqslant \rho t, \tag{2.12}$$

where $\| \ \|_2$ *denotes the norm defined by*

$$\| v \|_2^2 = h \sum_{j=0}^{\infty} |v_j|^2.$$

Proof. The idea is as follows: Let initial data be chosen equal to $1/a_{\max}$ times (2.10) near $x=0$, where $a_{\max}$ is the largest coefficient of (2.10) in absolute value, but cutting off smoothly to 0 for $jh \geqslant \varepsilon$. As time elapses, each smooth wave front will propagate rightwards at its group speed C_i. This will cause growth at least at fast as (2.12) if ρ is taken small enough. For rigorous proofs of various theorems of this kind, see [15, 16]. ∎

Theorems 1 and 2 are not quite the same as the GKS stability theorem. The latter asserts that even if every wave in (2.10) has $C=0$, the model is still unstable. From the point of view we have taken, it is not clear why this should be so, for if a cut off wave is set up as in the proof of Theorem 2, but with $C = 0$ for each component, then as t increases the wave front will approximately remain stationary. The explanation is that the GKS theorem does not define stability in terms of a simple l_2 norm, but in a more complicated fashion involving forcing data and solution values along the boundary, under which a wave that remains stationary at the boundary turns out to be *unstable* [10, Definition 3.3]. The GKS definition has other peculiarities too, the most troublesome of which is that it defines stability not in terms of a norm at a fixed time t, but in terms of an integral of the solution over all $t > 0$. We shall not go into the details.

The situation here is something like that discussed at the end of Section 1: by choosing a conservative definition of stability, one can obtain a theory that is robust with respect to variable coefficients, undifferentiated terms, and so on. In fact, a striking difference between the GKS theorem and our Theorem 1 (coupled with the G–R condition) is that the former gives a necessary *and sufficient* condition for stability, made possible by the use of the complicated norm. The difference between this situation and that of Section 1 is that in this case it is not as clear that for realistic computations, the conservative choice is generally necessary. There is reason to believe that the GKS definition may be realistic for problems involving inhomogeneous boundary data, but unrealistic for problems involving initial data alone. These details, however, are not yet well understood.

In practice, stability for a particular problem will be determined by a host of interacting phenomena that depend on whether and how smoothly the coefficients vary, whether an undifferentiated term is present, whether homogeneous or inhomogeneous boundary data are supplied, whether there is more than one boundary, and whether the boundaries are characteristic. Probably no simple theory can encompass all permutations of such effects without some artificiality. For further discussion of these matters, see [15, sect. 5].

3. Applications

We shall now give five examples of unstable boundary conditions, or their equivalents. In each case the unstable mode consists of nothing more than a combination of constant and sawtoothed signals; this is typical for instabilities encountered in practice. In the course of the examples we shall extend the theory to problems with interfaces and to multidimensional problems, where a vector group velocity becomes needed.

Because of the repeated occurence of sawtoothed waves, it is convenient to devise a name for schemes under which they propagate in the wrong direction.

Definition. Let Q be a scalar difference formula. Suppose that whenever Q admits a solution $v_j^n = z^n$ with $|z| = 1$ and group speed $C \in \mathbb{R}$, then it also admits the solution $v_j^n = (-1)^j z^n$, and this wave has group speed $C' \in \mathbb{R}$ satisfying $CC' \leqslant 0$, with $C' \neq 0$ if $C \neq 0$. Then Q is *x-reversing*. Likewise, if the existence of a solution $v_j^n = \kappa^j$ with $|\kappa| = 1$ and group speed C implies the existence of a solution $v_j^n = (-1)^n \kappa^j$ with $CC' \leqslant 0$, with $C' \neq 0$ if $C \neq 0$, then Q is *t-reversing*.

A difference formula based on the standard second-order centered difference in x or t will often be reversing for that variable, with $CC' = -1$. Thus LF, CN (Crank–Nicolson), and BE (backwards Euler) are x-reversing, and LF and LF4 (fourth-order leapfrog) are t-reversing, as is any modification of LF with (spatial) dissipation added. More generally, the general $(2l+1)$-point difference approximation to $\partial/\partial x$ or $\partial/\partial t$ of order $2l$ is also reversing [15], with $CC' < -1$ for $l \geqslant 2$. A dissipative scheme cannot be x-reversing, and a scheme that dissipates oscillations in t (for which there is no name) cannot be t-reversing [15].

APPLICATION 1 (Space extrapolation with t-reversing formulas). Let $u_t = u_x$ be modeled by a difference formula Q for $j \geqslant l$ coupled with q_jth-*order space extrapolation* boundary conditions

$$[(E-1)^{q_j} v^{n+1}]_j = 0 \qquad (0 \leqslant j \leqslant l-1) \tag{S}$$

for the boundary points, where E is the shift operator defined by $[Ev]_j = v_{j+1}$ and $q_j \geqslant 1$ for each j. The result appears in [10], and in various other papers, that S is unstable if $l = 1$ and the interior scheme is LF. Here is a generalization.

THEOREM 3. *Any consistent t-reversing difference formula Q for $u_t = u_x$, such as* LF *or* LF4 *with or without dissipation, is unstable in combination with the boundary condition S.*

Proof. The sawtoothed wave $v_j^n = (-1)^n$ satisfies S for any set $\{q_j\}$, and if Q is t-reversing, it also satisfies Q and has $C > 0$, since by consistency $v_j^n \equiv 1$ must satisfy Q with $C = -1 < 0$. By Theorem 1, the model is therefore unstable. ∎

The instability with S of an LF scheme with spatial dissipation added is pointed out in [9].

APPLICATION 2 ("One-sided leapfrog" with t-reversing formulas). Similarly, it has been noted in various papers that if $u_t = u_x$ is modeled by LF for $j \geqslant 1$ with the boundary condition

$$v_0^{n+1} = v_0^{n-1} + 2\lambda(v_1^n - v_0^n),$$

then the result is GKS-unstable. As a generalization, consider any set of boundary conditions

$$v_j^{n+1} = v_j^{n-1} + 2k\, D_j v_j^n, \qquad 0 \leqslant j \leqslant l-1, \tag{3.1}$$

where each D_j is a one-sided spatial difference operator involving at most j points to the left of center, consistent with $\partial/\partial x$. We obtain just as above

THEOREM 4. *Any consistent t-reversing difference formula Q for $u_t = u_x$ is unstable in combination with boundary condition* (3.1).

APPLICATION 3 (Sign-changing coefficients; nonlinear instability). Consider the problem

$$\begin{aligned} u_t &= a_- u_x \qquad (x < 0), \\ &= a_+ u_x \qquad (x > 0), \end{aligned} \tag{3.2}$$

where a_- and a_+ are constants. To model this by finite differences, we might set up a grid $((j+\frac{1}{2})h, nk)$ for $-\infty < j < \infty$, $n \geqslant 0$. Suppose we apply consistent difference formulas Q_- and Q_+ for $x \leqslant -h/2$ and $x \geqslant h/2$, respectively, taking no special measures to improve accuracy at the interface. The stability question for such an interface is essentially the same as for an initial boundary value problem, and the GKS theory has been applied to such problems by Kreiss, Ciment, Oliger, and others [6]. Formally, a scalar model including an interface can be "folded" into an initial boundary value problem for a system of two variables, and then the GKS theory is directly applicable. What is really going on in such a process is a search for eigensolutions or generalized eigensolutions consisting of waves that are *outgoing* from the point of view of the interface. That is, *a difference model involving a scheme- or mesh-change interface is* GKS-*stable if and only if there is no eigensolution of the kind suggested in Fig.* 3.

If $\operatorname{sgn} a_- = \operatorname{sgn} a_+$, then most models for (3.2) are stable, but stability often vanishes if $\operatorname{sgn} a_- \neq \operatorname{sgn} a_+$.

THEOREM 5. *Let* (3.2) *be modeled by consistent formulas Q_- and Q_+ as indicated above. If $a_- > 0 > a_+$, the model is unstable. If $a_- < 0 < a_+$ and Q_- and Q_+ are both x-reversing or both t-reversing, the model is also unstable.*

Proof. In the first case, the constant function $v_j^n \equiv 1$ is an outgoing wave that

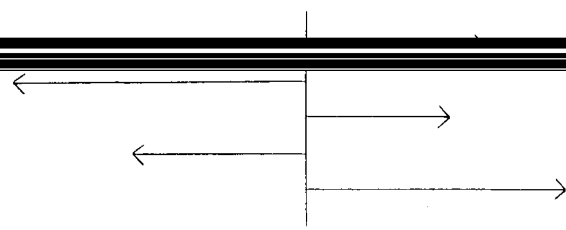

FIG. 3. In a problem containing an interface, a solution consisting of a set of outgoing waves on each side will be unstable.

satisfies all the difference formulas, so the model is unstable by Theorem 1. In the second case, the same is true for a space or time sawtooth $(-1)^j$ or $(-1)^n$. ▮

This elementary example is related to certain known examples of *nonlinear instability*. If the Burgers equation

$$u_t = uu_x$$

is modeled by the LF scheme

$$v_j^{n+1} - v_j^{n-1} = \lambda v_j^n (v_{j+1}^n - v_{j-1}^n),$$

then exponentially growing instabilities arise that are characterized by oscillations of the form [8, 11]

$$v_j^n \approx 0, \qquad v_{j+1}^n < 0, \qquad v_{j+2}^n > 0, \qquad v_{j+3}^n \approx 0.$$

Though it is easy enough to examine this problem directly, it also has a rough interpretation along GKS lines: LF is an x-reversing formula, and the instability observed looks approximately like the outgoing sawtooth of Theorem 5 from the point of view of the sign-change interface at $x_{j+3/2}$. The linear growth of this outgoing wave would be converted into exponential by reflection at points x_j and x_{j+3} even if the coefficients v_j did not change from one time step to the next; the fact that they do makes the growth still more rapid.

APPLICATION 4 (Mesh refinement). In problems where the solution is smoother in some regions than in others, it may be useful to combine grids of various sizes [6]. Where two such grids meet, some kind of interface condition will be required. Here is a mesh refinement scheme for which the stability result takes a particularly interesting form (Joseph Oliger, private communication). Suppose that for $x \geqslant 0$, the grid $x_j = hj$ $(j \geqslant 0)$ is set up, while for $x \leqslant 0$, this is coarsened by an integral factor of $m \geqslant 2$, so that the grid is $x_j = mhj$ for $j \leqslant 0$. If $u_t = u_x$ is modeled by LF for $j \leqslant -1$, a formula is still needed to determine v_0^n. The obvious choice is to apply the coarse grid LF formula at $j = 0$, which is possible because the value required at $x = mh$ is available from the fine grid,

$$v_0^{n+1} = v_0^{n-1} + m\lambda(v_m^n - v_{-1}^n). \tag{3.3}$$

Now suppose a wave is considered of the form

$$v_j^n = (-1)^j \quad (j \geqslant 0), \qquad = 1 \quad (j \leqslant 0). \tag{3.4}$$

On $x \leqslant 0$, this wave is constant and has $C = -1$. On $x \geqslant 0$, it is sawtoothed and has $C > 0$ since LF is x-reversing. Thus (3.4) is outgoing on both sides of the interface. Moreover *if m is even*, it obviously satisfies (3.3), so we have instability.

This conclusion can be generalized as

THEOREM 6. *Let $u_t = u_x$ be modeled by a consistent x-reversing 3-point formula on $x_j = jh$ for $j \geqslant 1$ coupled with any consistent formula on $x_j = jmh$ for $j \leqslant 0$, with right-hand values for the latter near the interface taken where needed from points imh with $i \geqslant 1$. Then if m is even, the model is unstable.*

For LF or CN the sawtooth of Eq. (3.4) turns out to be the only instability that arises, so this kind of mesh refinement is stable if m is odd.

APPLICATION 5 (Two-dimensional problems). Abarbanel and Gottlieb [1] and Abarbanel and Murman [2] have studied the stability of various difference schemes for the following problem in two space dimensions:

$$u_t = u_x + u_y, \qquad x, t \geqslant 0, \quad y \in (-\infty, \infty). \tag{3.5}$$

The solutions to this equation consist of functions

$$u(x, y, t) = u(x + t, y + t, 0).$$

That is, information propagates with a vector velocity $(-1, -1)$. Since the flow is outward across the boundary $x = 0$, no boundary conditions should be given there.

For a multidimensional problem like this, ξ becomes a wave number vector $\boldsymbol{\xi}$, and the group speed (1.7) generalizes to a vector *group velocity* given by

$$\mathbf{C} = \nabla_{\xi} \omega, \tag{3.6}$$

where ∇_{ξ} denotes the gradient with respect to $\boldsymbol{\xi}$. As in the one-dimensional case, difference schemes not only lead to incorrect group speeds, but may cause propagation in the wrong direction—which means at any angle in the (x, y) plane whatsoever. See [14] for a discussion with examples. In two dimensions, Theorem 1 becomes: *if a difference model of* (3.5) *admits a solution consisting of waves with group velocity* $\mathbf{C}$ *pointing into* $x \geqslant 0$ (*i.e., with* $C_x \geqslant 0$), *it is unstable.* If one such wave has $C_x > 0$, then unbounded growth in l_2 will take place, as in Theorem 2.

For example, suppose (3.5) is modeled by the leapfrog formula

$$v_{ij}^{n+1} - v_{ij}^{n-1} = \lambda(v_{i+1,j}^n - v_{i-1,j}^n) + \lambda(v_{i,j+1}^n - v_{i,j-1}^n). \tag{3.7}$$

The dispersion relation for this scheme is

$$\sin \omega k = -\lambda \sin \xi h - \lambda \sin \eta h,$$

where $\boldsymbol{\xi} = (\xi, \eta)$, and from (3.6) there follow the group velocity components

$$C_x = -\cos \xi h / \cos \omega k, \qquad C_y = -\cos \eta h / \cos \omega k.$$

As usual, these reduce to the ideal value $\mathbf{C} = (-1, -1)$ for ξh, $\omega k \approx 0$. If we look at parasites, on the other hand, we see that a sawtooth form in x or y negates C_x or C_y, respectively, and a sawtooth in t negates both. One has

(a) $(\xi h, \eta h, \omega k) = (0, 0, 0), (\pi, \pi, \pi)$ $\quad \mathbf{C} = (-1, -1)$,
(b) $(\xi h, \eta h, \omega k) = (\pi, 0, 0), (0, \pi, \pi)$ $\quad \mathbf{C} = (+1, -1)$,
(c) $(\xi h, \eta h, \omega k) = (0, \pi, 0), (\pi, 0, \pi)$ $\quad \mathbf{C} = (-1, +1)$,
(d) $(\xi h, \eta h, \omega k) = (\pi, \pi, 0), (0, 0, \pi)$ $\quad \mathbf{C} = (+1, +1)$.

Thus parasites can travel in any of the directions at 45° to the grid. If any parasite of form (b) or (d) is permitted by the boundary conditions, the difference model is unstable.

Abarbanel *et al.* consider various boundary formulas. Four of these are *space extrapolation* and *skewed space extrapolation*,

$$(E_x - 1)^q v_0^{n+1} = 0, \tag{S}$$

$$(E_x E_y - 1)^q v_0^{n+1} = 0, \tag{SS}$$

and *space–time extrapolation* and *skewed space–time extrapolation*,

$$(E_x E_t^{-1} - 1)^q v_0^{n+1} = 0, \tag{ST}$$

$$(E_x E_y E_t^{-1} - 1)^q v_0^{n+1} = 0. \tag{SST}$$

Here E_x, E_y, and E_t denote the shift operators in x, y, and t. By counting sign changes, one can see which boundary formulas permit which sawtooths. One finds:

	stable	*unstable*
S	$(0, 0, 0), (0, \pi, 0)$	$(0, 0, \pi), (0, \pi, \pi)$
SS	$(0, 0, 0), (\pi, \pi, \pi)$	$(0, 0, \pi), (\pi, \pi, 0)$
ST	$(0, 0, 0), (0, \pi, 0), (\pi, 0, \pi), (\pi, \pi, \pi)$	
SST	$(0, 0, 0), (\pi, 0, \pi)$	$(0, \pi, \pi), (\pi, \pi, 0)$.

Thus S, SS, *and* SST *are all unstable with LF.* It turns out that ST, which we see has no sawtooth instabilities, is indeed stable.

Other difference formulas typically permit fewer sawtooths, hence are stable with more boundary conditions. Let us generalize to d space dimensions. If $\boldsymbol{\kappa}$ and $\mathbf{j}$ are d-vectors, $\boldsymbol{\kappa}^{\mathbf{j}}$ will denote $\kappa_1^{j_1} \cdots \kappa_d^{j_d}$.

DEFINITION. Let Q be a scalar difference formula in d space dimensions. Suppose that whenever Q admits a solution $v_{\mathbf{j}}^n = \boldsymbol{\kappa}^{\mathbf{j}} z^n$ with $|z| = |\kappa_i| = 1$ for each i, $\kappa_I = 1$ for some I, and group velocity $\mathbf{C} \in \mathbb{R}^d$, then it also admits the solution $v_{\mathbf{j}}^n = (-1)^I \boldsymbol{\kappa}^{\mathbf{j}} z^n$, and this wave has group velocity $\mathbf{C}' \in \mathbb{R}^d$ satisfying $C_i' = C_i$ for $i \neq I$ and $C_I C_I' \leqslant 0$, with $C_I' \neq 0$ if $C_I \neq 0$. Then Q is x_I-*reversing*. Suppose that whenever Q admits a solution $v_j^n = \boldsymbol{\kappa}^j$ with $|\kappa_i| = 1$ for all i and group velocity $\mathbf{C} \in \mathbb{R}^d$, then it also admits the solution $v_j^n = \boldsymbol{\kappa}^j(-1)^n$, with group velocity $\mathbf{C}' \in \mathbb{R}^d$ satisfying $C_i C_i' \leqslant 0$ for $1 \leqslant i \leqslant d$, with $C_i' \neq 0$ if $C_i \neq 0$. Then Q is *t-reversing.*

Now let Q be a difference model of

$$u_t = \sum_{j=1}^{d} u_{x_j}$$

on $t, x_1 \geqslant 0$, $x_j \in (-\infty, \infty)$ for $2 \leqslant j \leqslant d$, and let the boundary conditions S, SS, ST, SST be extended in the obvious way. By the same arguments as above we obtain

THEOREM 7. *(The following assertions hold in the stated direction only; their converses are not in general valid).*

(i) *The model* S, Q *is unstable if* Q *is t-reversing.*

(ii) *The model* SS, Q *is unstable if* Q *is t-reversing or if* Q *is* x_1*-reversing and also* x_j*-reversing for at least one* $j \geqslant 2$.

(iii) *The model* SST, Q *is unstable if* Q *is* x_1*-reversing and/or t-reversing, and also* x_j*-reversing for at least one* $j \geqslant 2$.

Among the formulas Q considered by Abarbanel *et al.* are multidimensional versions of LF, CN, BE, and MC (MacCormack's scheme). One sees readily that LF is t-reversing and x_j-reversing for each j, CN and BE are x_j-reversing for each j but not t-reversing, and MC is not reversing in any variable. It turns out that almost all combinations of these schemes with S, SS, ST, or SST that are not ruled unstable by Theorem 7 are in fact stable. The exception is CN with ST in the case $\lambda \geqslant 2$, which Beam *et al.* have shown has a generalized eigensolution that is not a simple sawtooth [3].

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Notes added in proof. (a) A rigorous application of the ideas of this paper to the derivation of unstable growth rates in l_2 norms will appear in [16]. That paper also investigates the relationship of instability to infinite reflection coefficients, which was mentioned here only in passing. (b) The problem of instability for difference models with boundaries is closely related to the problem of ill-posedness of multidimensional differential equations with boundaries. An algebraic theory for the latter problem was derived by Kreiss and others around 1970, and will be described from the group velocity point of view in a forthcoming paper by Robert Higdon.

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