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On spurious reflections, nonuniform grids and finite difference discretizations of wave equations

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2000 Mathematics Subject Classification: 65M06, 65M50
Keywords and Phrases: wave equations, finite difference methods, nonuniform grids, spurious reflections, box scheme
Note: Work carried out under project MAS1.3 - `Numerical Methods for Applications in PDEs.' Funding for JF from an NWO Innovative Research Grant is gratefully acknowledged.

On spurious reflections, nonuniform grids and finite difference discretizations of wave equations

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ABSTRACT

This paper addresses nonphysical reflections encountered in the discretization of wave equations on nonuniform grids. Such nonphysical solutions are commonly attributed to spurious modes in the numerical dispersion relation. We provide an example of a discretization in which a (nonspurious) physical mode is spuriously energized at a grid nonuniformity. It is found that, in particular, the box scheme and, in general, certain discretizations within the class of Runge-Kutta methods, are free from such spurious reflections.

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The central difference discretization of the scalar advection equation suffers from spurious numerical reflections on nonuniform grids, as is well-documented [5, 11, 10]. See especially the excellent review of Trefethen [9], where the numerical dispersion relation is studied, and where the numerical group velocity is identified as the propagation speed of spurious, reflected waves. Specifically, it is observed that the numerical dispersion relation for central differencing on a uniform grid supports, for each frequency ω, two wave numbers κ having opposite group velocities. For a solution involving only a single frequency, only these wave numbers can be active. Vichnevetsky [11] has shown that the spurious wave number is excited at an interface between two regions with uniform but unequal mesh spacing.

Much of the literature assumes the point of view that spurious solution modes and nonphysical reflections in finite difference methods are unavoidable. Sometimes artificial diffusion is used to severely damp high frequency modes. In this paper we expound on the phenomenon of spurious reflections on nonuniform grids. In the first place we see that spurious reflections are not unavoidable; any Runge-Kutta method applied to the spatial derivative of the advection equation will result in a dispersion relation with only a single root. For a subclass of RK methods, we prove that the dispersion relation is monotone. Second, we show that for higher order derivatives, or for systems of PDEs, the existence of spurious modes is not a necessary condition for reflections. The staggered discretization of the wave equation experiences an artificial excitation of physical solution modes at a change in grid spacing. We show that such spurious coupling of physical modes is impossible for spatial discretizations within the class of Runge-Kutta methods.

The paper is organized as follows:

In §1 we review the well-documented example of the *advection equation*, discretized by central finite differences. Our analysis is essentially a review of that of Vichnevetsky [11]. For this case,

the reflections generated by a change in grid spacing are a manifestation of spurious modes present in the dispersion relation.

By contrast, the box scheme has been shown to be free of spurious modes [1]. Consequently, in §2 we show that the box scheme incurs no reflections for the advection equation on a nonuniform grid. More generally, any Runge-Kutta method, when used to approximate the spatial derivative of the advection equation, is free of spurious modes, and we prove that any RK method whose stability function is a diagonal Padé approximation has a monotone dispersion relation.

In §3 we continue the investigation for the *wave equation*, using a staggered central discretization, which has no spurious modes. Nevertheless, reflections are again observed, but here *physical solution modes* are spuriously excited at a point of grid refinement.

The box scheme discretization is also reflection-free for the wave equation. The analysis of §4 reveals that the important property of the box scheme in this regard is that the resulting semi-discretized system, when written as a one-step recursion in space, may be globally decoupled into recursions for the characteristics.

In §5 we generalize the above observations and identify a class of Runge-Kutta methods, applied to the spatial derivative of systems of linear hyperbolic PDEs, as being reflection-free.

1. Central difference discretization of the advection equation

In this section and the following, we consider the advection equation

$$u_t + cu_x = 0 \tag{1.1}$$

on the real line with uniform propagation speed $c > 0$. Substituting the plane wave solution $u = \exp \mathrm{i}(\kappa x - \omega t)$ into (1.1) gives the dispersion relation [12]

$$\omega = c\kappa, \tag{1.2}$$

which is the dotted line in the left plot of Figure 1.1. The slope of the dispersion relation is the group velocity

$$\frac{d\omega}{d\kappa} = c,$$

which is constant and positive. Since all wavelengths move with the same velocity, a given signal propagates to the right unchanged with velocity c.

It is also possible to derive the dispersion relation of a numerical approximation. In general, numerical methods are dispersive even when the PDE to be discretized is not so, and the numerical group velocity is a function of the wavelength κ. In this case, an initial signal will change shape due to dispersion.

Throughout this paper we work with semidiscretizations, i.e. assuming continuity in time. This primarily saves superfluous notation. Furthermore, any choice of a time integrator would be rather arbitrary. However, numerical reflections can be introduced as easily through the time integrator as through the spatial discretization. See the comments in the Conclusions. Since time is taken continuous, we are mostly interested in the inverse dispersion relation $\kappa(\omega)$ for which the group velocity is $(d\kappa/d\omega)^{-1}$.

The analytical dispersion relation (1.2) associates one wavenumber κ to each frequency ω. Some discretizations may associate more wave numbers to a frequency than the analytical solution. In this case we say the numerical solution admits *spurious modes*.

The central difference discretization of (1.1) is

$$\dot{u}_j + c\frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}} = 0, \tag{1.3}$$

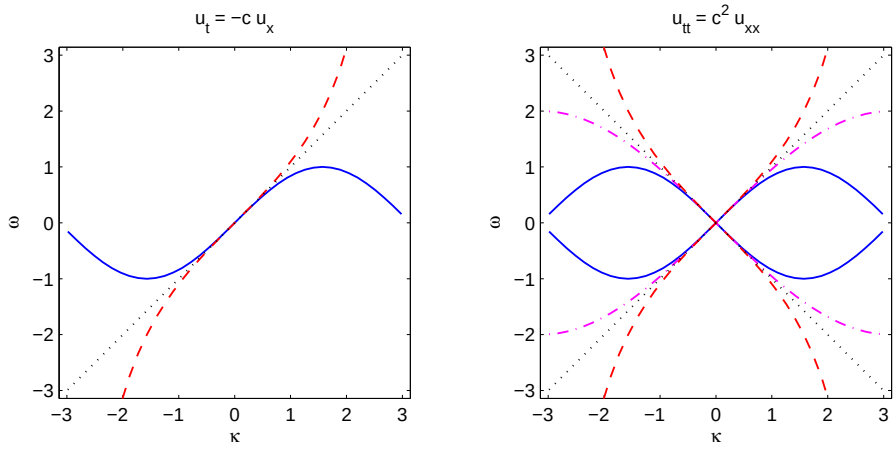

Figure 1.1: Dispersion relations of the exact solution ($\cdots$), central difference (—) and box (- - -) schemes, for (left) the advection and (right) wave equations for $c \equiv h \equiv 1$. The dispersion relation of the staggered central discretization of the wave equation is also shown (- · -).

and it is well-known that this discretization supports modes with spurious negative group velocity, which, even if not initially present, will be activated when a signal encounters a change in grid spacing [11]. To see this, we follow Vichnevetsky's [11] reasoning and apply a time-Fourier transformation

$$u_j(t) = \int_{-\infty}^{\infty} e^{-\mathrm{i}\omega t}\hat{u}_j(\omega)\, d\omega \tag{1.4}$$

to yield the difference equation

$$-\mathrm{i}\omega\hat{u}_j + c\frac{\hat{u}_{j+1} - \hat{u}_{j-1}}{x_{j+1} - x_{j-1}} = 0.$$

Let us introduce the equivalent one-step method

$$\hat{U}_{j+1} = S(\mathrm{i}\omega\bar{h}_j/c)\hat{U}_j, \quad \hat{U}_j := \begin{pmatrix} \hat{u}_j \\ \hat{u}_{j-1} \end{pmatrix}, \quad S(z) = \begin{bmatrix} 2z & 1 \\ 1 & 0 \end{bmatrix}, \tag{1.5}$$

where $\bar{h}_j = (x_{j+1} - x_{j-1})/2$ and we assume $|\omega h_j/c| < 1$. The matrix $S(z)$ can be diagonalized:

$$S(z) = X(z)D(z)X(z)^{-1}, \quad X(z) = \begin{bmatrix} z + \sqrt{1+z^2} & z - \sqrt{1+z^2} \\ 1 & 1 \end{bmatrix},$$

where $D(z)$ is a diagonal matrix containing the eigenvalues of $S(z)$, i.e. the roots of its characteristic polynomial,

$$\lambda^{\pm}(S(z)) = z \pm \sqrt{1+z^2}. \tag{1.6}$$

The dispersion relation is obtained for a uniform grid $\bar{h}_j \equiv h$ by inserting the plane wave solution $\hat{u}_{j+1} = e^{\mathrm{i}\kappa h}\hat{u}_j$ in (1.5). Since there are two roots (1.6), there are two solutions

$$\exp(\mathrm{i}\kappa^{\pm}h) = \lambda^{\pm}(S(\mathrm{i}\omega h/c)).$$

The dispersion relation for (1.3),

$$\omega = \frac{c}{h}\sin\kappa h,$$

is the solid line in the left plot of Figure 1.1. To each $|\omega h/c| < 1$, there correspond two roots $\kappa^{\pm}$ with opposite slope. The group velocity [12] is given by the slope of the dispersion relation,

$$\frac{d\omega}{d\kappa} = c\cos\kappa h,$$

and this allows us to identify the roots (1.6) corresponding to right and left group velocities:

$$\begin{aligned} e^{\mathrm{i}\kappa^+ h} &= R(\mathrm{i}\omega\bar{h}_j/c), \qquad R(z) = z + \sqrt{1+z^2}, \\ e^{\mathrm{i}\kappa^- h} &= L(\mathrm{i}\omega\bar{h}_j/c), \qquad L(z) = z - \sqrt{1+z^2}, \end{aligned}$$

and $D(z) = \mathrm{diag}(R(z), L(z))$.

Furthermore, on a uniform grid the j dependence may be dropped from $D(\mathrm{i}\omega h/c)$ and $X(\mathrm{i}\omega h/c)$, and the recursion (1.5) premultiplied by $X(\mathrm{i}\omega h/c)^{-1}$ to give two decoupled characteristic solutions

$$\hat{C}_{j+1} = D(\mathrm{i}\omega h/c)\hat{C}_j, \quad \hat{C}_j := X(\mathrm{i}\omega h/c)^{-1}\hat{U}_j = \begin{pmatrix} \hat{r}_j \\ \hat{\ell}_j \end{pmatrix} \quad \Rightarrow \quad \begin{cases} \hat{r}_{j+1} = R(\mathrm{i}\omega h/c)\hat{r}_j \\ \hat{\ell}_{j+1} = L(\mathrm{i}\omega h/c)\hat{\ell}_j \end{cases}.$$

That is, central differencing supports both right and (spurious) left characteristic group velocities, and on a uniform grid these are everywhere decoupled.

Next consider a grid with two regions of uniform but different spacing ($h^I \neq h^{II}$)

$$x_j = \begin{cases} jh^I, & j < 0 \\ jh^{II}, & j \geq 0 \end{cases}. \tag{1.7}$$

Away from the interface at $x_0 = 0$, the grid spacing is uniform, and the right and left characteristics decouple as previously noted. Let us denote $S_j = S(\mathrm{i}\omega\bar{h}_j/c)$, $X_j = X(\mathrm{i}\omega\bar{h}_j/c)$, and similarly for D_j, R_j and L_j. Then, applying (1.5) twice across the interface gives

$$\hat{U}_1 = S_0 S_{-1}\hat{U}_{-1},$$

or

$$\hat{C}_1 = X_1^{-1}X_0 D_0 X_0^{-1}X_{-1}D_{-1}\hat{C}_{-1}, \tag{1.8}$$

and in general the right and left characteristics couple, resulting in a reflection. Note that (for this example)

$$X_j = \begin{bmatrix} R_j & L_j \\ 1 & 1 \end{bmatrix}.$$

Denoting $R^I = R(\mathrm{i}\omega h^I/c)$, etc., let us invert (1.8) to find $\hat{C}_{-1}$

$$\begin{pmatrix} \hat{r}_{-1} \\ \hat{\ell}_{-1} \end{pmatrix} = \begin{bmatrix} R_{-1} & 0 \\ 0 & L_{-1} \end{bmatrix}^{-1} \begin{bmatrix} R_{-1} & L_{-1} \\ 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} R_0 & L_0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} R_0 & 0 \\ 0 & L_0 \end{bmatrix}^{-1} \begin{bmatrix} R_0 & L_0 \\ 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} R_1 & L_1 \\ 1 & 1 \end{bmatrix} \begin{pmatrix} \hat{r}_1 \\ \hat{\ell}_1 \end{pmatrix}.$$

If we assume there is a right-moving wave in $\{x < 0\}$ and no left-moving wave in $\{x \geq 0\}$, i.e. set $\hat{\ell}_1 = 0$ in the above, then we can solve for the reflection ratio $\rho := \hat{\ell}_{-1}/\hat{r}_{-1}$, to give

$$\rho = -\frac{R_{-1}}{L_{-1}}\left(\frac{R_{-1}(R_0 - R_1 + L_0) - R_0 L_0}{L_{-1}(R_0 - R_1 + L_0) - R_0 L_0}\right),$$

which is nonzero in general. In other words, $\hat{\ell}_{-1}$ will be nonzero even when $\hat{\ell}_1 = 0$; the spurious left characteristic on $\{x < 0\}$ is excited due to the grid nonuniformity.

2. Box scheme discretization of the advection equation

The box scheme has recently received a lot of attention in the context of wave equations, due to the discovery of its multisymplecticity [4, 8]. Ascher & McLachlan have shown that the box scheme has no spurious modes [1]. Based on the considerations of the previous section, it then comes as no surprise that the box scheme is free from spurious reflections.

For the advection equation (1.1) the box scheme is

$$\frac{\dot{u}_j + \dot{u}_{j+1}}{2} + c\frac{u_{j+1} - u_j}{x_{j+1} - x_j} = 0 \tag{2.1}$$

After time-Fourier transformation (1.4), this scheme gives the recursion (with $h_j := x_{j+1} - x_j$)

$$\hat{u}_{j+1} = R(\frac{\mathrm{i}\omega h_j}{c})\hat{u}_j, \qquad R(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}.$$

The dispersion relation is obtained for a uniform grid by inserting the plane wave solution $\hat{u}_{j+1} = e^{\mathrm{i}\kappa h}\hat{u}_j$, which gives

$$e^{\mathrm{i}\kappa h} = R(\frac{\mathrm{i}\omega h}{c}) \quad \Rightarrow \quad \frac{\omega h}{2c} = \frac{1 - e^{\mathrm{i}\kappa h}}{1 + e^{\mathrm{i}\kappa h}},$$

i.e.,

$$\omega(\kappa) = \frac{2c}{h}\tan\frac{\kappa h}{2}.$$

Taking the derivative with respect to κ yields a positive group velocity for all κ, see Figure 1.1 (left). Since the box scheme supports only right-moving groups, there can be no reflections.

What properties of the box scheme prevent the generation of spurious reflections? In the first place, the box scheme has a compact stencil: it is a one-step method, and therefore has only one root. Secondly, the dispersion relation is monotone, as implied by the result of Ascher & McLachlan [1]. In the following we consider a generalization of the box scheme to Runge-Kutta spatial discretizations.

It is straightforward to apply a Runge-Kutta method (see e.g. [7]) to the spatial derivative of (1.1). We write

$$u_x = -c^{-1}u_t,$$

and simply apply the RK method as for an initial value problem to obtain the relation between grid points j and $j+1$. For an s-stage RK method with coefficients a_{ik}, b_i, $i, k = 1, \ldots, s$:

$$\begin{aligned} &U_i = -c^{-1}\partial_t(u_j + h_j\textstyle\sum_{k=1}^{s} a_{ik}U_k), \quad i = 1, \ldots, s \\ &u_{j+1} = u_j + h_j\textstyle\sum_{i=1}^{s} b_i U_i. \end{aligned} \tag{2.2}$$

Substituting the plane wave solution $u_j(t) = \exp\mathrm{i}(\kappa h j - \omega t)$ into (2.2) yields the numerical dispersion relation

$$e^{\mathrm{i}\kappa h} = R(\mathrm{i}\omega h/c). \tag{2.3}$$

Here, $R(z)$ is the stability function associated with a Runge-Kutta method having coefficients $b = (b_i)$, $A = (a_{ik})$, i.e.

$$R(z) = 1 + zb^T(I - zA)^{-1}e, \tag{2.4}$$

where $e = (1, \ldots, 1)^T$, see [7].

For any $\tilde{\omega} = \omega h/c$, the right side of (2.3) evaluates to some point in the complex plane. If the discretization is nondamping, then $R(\mathrm{i}\tilde{\omega})$ is a point on the unit circle, and (2.3) defines a unique $\kappa h \in (-\pi, \pi]$ (for methods with damping, it is the real part of κh—also uniquely determined in this interval—that plays a role in the dispersion relation). In other words, for each $\tilde{\omega}$ there can be only one corresponding κh, so Runge-Kutta methods have only one root.

For the special case in which the stability function $R(z)$ is a diagonal Padé approximation, we can prove that the dispersion relation is monotone (i.e. the group velocity is always positive for positive c):

Theorem 2.1 *Suppose the stability function $R(z)$ of a Runge-Kutta method is given by the (p,p)-Padé approximation of the exponential function. If this function is used to discretize the advection equation in space, then the numerical dispersion relation will be real-valued (that is, the discretization is nondiffusive) and monotone. In particular, the group velocity is everywhere positive.*

Proof. The diagonal (p,p)-Padé approximation of the exponential function can be written as a ratio of Hankel functions (see Driver & Temme [6])[1]

$$\exp(z) \approx R(z) := -\exp(z)\frac{H^{(1)}_{p+1/2}(-\mathrm{i}z/2)}{H^{(2)}_{p+1/2}(-\mathrm{i}z/2)}. \tag{2.5}$$

The Hankel functions $H^{(1)}_{p+1/2}$ and $H^{(2)}_{p+1/2}$ are a complex conjugate pair. In terms of modulus $M_{p+1/2}$ and phase $\theta_{p+1/2}$ (see [2], 9.2.17)

$$H^{(1)}_{p+1/2}(z) = M_{p+1/2}(z)\exp(\mathrm{i}\theta_{p+1/2}(z)), \qquad H^{(2)}_{p+1/2} = M_{p+1/2}(z)\exp(-\mathrm{i}\theta_{p+1/2}(z)),$$

and (2.5) simplifies, for $z = \mathrm{i}\tilde{\omega} = \mathrm{i}\omega h/c$, to

$$R(\mathrm{i}\tilde{\omega}) = -\exp(\mathrm{i}\tilde{\omega})\exp(-2\mathrm{i}\theta_{p+1/2}(\tilde{\omega}/2)),$$

from which follows that $|R(\mathrm{i}\tilde{\omega})| = 1$ and the method is nondiffusive.

Writing $\exp(\mathrm{i}\tilde{\kappa}) = R(\mathrm{i}\tilde{\omega})$, where $\tilde{\kappa} = \kappa h$, the (inverse) dispersion relation becomes

$$\tilde{\kappa}(\tilde{\omega}) = \tilde{\omega} - 2\theta_{p+1/2}(\tilde{\omega}/2) - \pi.$$

Furthermore, from [2] 9.2.21 the derivative of the phase is given by

$$\theta'_{p+1/2}(\tilde{\omega}) = \frac{2}{\pi\tilde{\omega}}M^{-2}_{p+1/2}(\tilde{\omega}),$$

where from [2] 10.1.27,

$$M^2_{p+1/2}(\tilde{\omega}) = \frac{2}{\pi\tilde{\omega}}\sum_{k=0}^{p}\frac{(2p-k)!(2p-2k)!}{k![(p-k)!]^2}(2\tilde{\omega})^{2p-2n} = 1 + \frac{\alpha_{p-1}}{\tilde{\omega}^2} + \cdots\frac{\alpha_0}{\tilde{\omega}^{2p}},$$

and all of the α_j are positive. As a result,

$$\theta'_{p+1/2}(\tilde{\omega}) = \frac{1}{1 + \frac{\alpha_{p-1}}{\tilde{\omega}^2} + \cdots\frac{\alpha_0}{\tilde{\omega}^{2p}}},$$

and $\theta'_{p+1/2}$ is symmetric about $\tilde{\omega} = 0$ and increases monotonically from $\theta'_{p+1/2}(0) = 0$ to $\theta'_{p+1/2}(+\infty) = 1$. It follows that the group velocity, whose inverse is

$$\tilde{\kappa}'(\tilde{\omega}) = 1 - \theta'_{p+1/2}(\tilde{\omega}/2),$$

[1] We thank Nico Temme for suggesting this proof.

is everywhere positive. □

Therefore, any Runge-Kutta spatial discretization with stability function on the diagonal of the Padé table will be free of spurious reflections. In particular, the Gauss, Lobatto IIIA and Lobatto IIIB schemes have this property [7].

At this point it is tempting to conclude that reflections are simply a manifestation of spurious modes in the numerical dispersion relation of a given discretization. However, the situation is more complicated when considering *systems* of PDEs or higher order derivatives. This situation will be illustrated in the next two sections using the simple example of the wave equation, written as a system of two first order PDES, and discretized by the staggered central and box schemes, neither of which has spurious modes in the dispersion relation. Nonetheless, we will see that the staggered discretization suffers from reflections, whereas the box scheme does not.

3. Staggered central discretization of the wave equation

In this section and the following, we consider the wave equation written as a pair of first order PDEs

$$u_t = cv_x, \qquad v_t = cu_x. \tag{3.1}$$

The exact dispersion relation

$$\omega = \pm c\kappa,$$

shown as a dotted line on the right plot in Figure 1.1, associates two wave numbers to each frequency.

Central differencing applied to (3.1) gives

$$\dot{u}_j = c\frac{v_{j+1} - v_{j-1}}{x_{j+1} - x_{j-1}}, \qquad \dot{v}_j = c\frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}}$$

The numerical dispersion relation has spurious modes: specifically, there are four wave numbers κ corresponding to each frequency $|\omega| < c/h$, see Figure 1.1.

Instead we consider an improved discretization, obtained by staggering u and v. Let $u_j \approx u(x_j)$ and $v_{j+1/2} \approx v(x_j + h_j/2)$, where $h_j = x_{j+1} - x_j$. Define the staggered central discretization

$$\dot{u}_j = \frac{c}{\bar{h}_j}(v_{j+1/2} - v_{j-1/2}), \qquad \dot{v}_{j+1/2} = \frac{c}{h_j}(u_{j+1} - u_j), \tag{3.2}$$

where $\bar{h}_j = (h_j + h_{j-1})/2$. On a uniform grid, $h \equiv h_j \equiv \bar{h}_j$, this discretization reduces to the standard three-point approximation of the Laplacian

$$\ddot{u}_j = \frac{c^2}{h^2}(u_{j+1} - 2u_j + u_{j-1}). \tag{3.3}$$

The numerical dispersion relation,

$$\omega = \pm\frac{2c}{h}\sin^2\frac{\kappa h}{2},$$

is shown in Figure 1.1. It has no spurious roots. Yet, as illustrated in Figure 3.1 on the left, a numerical simulation of a right-translating pulse, computed using (3.2) on a grid (1.7) with $h^I/h^{II} = 7$, clearly incurs reflections at the interface x_0.

We adapt the analysis of §1. Transforming in time according to (1.4), let $\hat{U}_j := (\hat{u}_j, \hat{v}_{j-1/2})^T$. The recursion analogous to (1.5) is

$$\hat{U}_{j+1} = S_j\hat{U}_j, \qquad S_j = \begin{bmatrix} 1 - \omega^2 h_j\bar{h}_j c^{-2} & -\mathrm{i}\omega h_j c^{-1} \\ -\mathrm{i}\omega\bar{h}_j c^{-1} & 1 \end{bmatrix}. \tag{3.4}$$

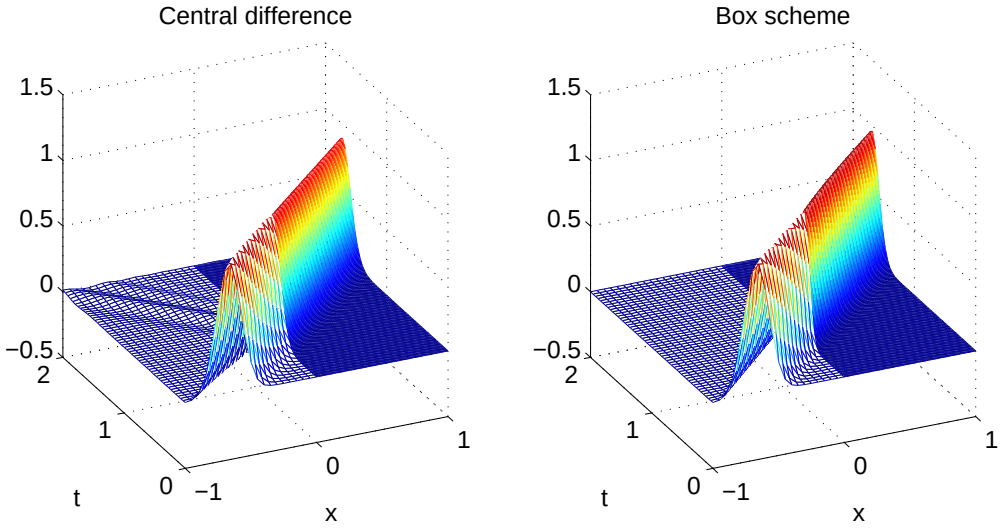

Figure 3.1: Pulse entering a region of mesh refinement, for (left) staggered central differencing and (right) box schemes.

The roots of S_j corresponding to the right and left characteristics in the dispersion relation are

$$R_j = R(\mathrm{i}\omega c^{-1}\sqrt{h_j\bar{h}_j}), \qquad R(z) = 1 - \frac{1}{2}z^2 + \sqrt{z^4/4 + z^2},$$
$$L_j = L(\mathrm{i}\omega c^{-1}\sqrt{h_j\bar{h}_j}), \qquad L(z) = 1 - \frac{1}{2}z^2 - \sqrt{z^4/4 + z^2},$$

and S_j can be diagonalized as before (assuming $\omega^2 h_j\bar{h}_j/c^2 < 4$)

$$S_j = X_j D_j X_j^{-1}, \quad X_j = \begin{bmatrix} \frac{\mathrm{ic}}{\omega h_j}R_j & \frac{\mathrm{ic}}{\omega h_j}L_j \\ 1 & 1 \end{bmatrix}.$$

where $D_j := \mathrm{diag}(R_j, L_j)$.

As before we can define characteristic variables $\hat{C}_j := X_j^{-1}\hat{U}_j$, where $\hat{C}_j = (\hat{r}_j, \hat{\ell}_j)$, and for the grid (1.7), the recursion (1.8) again holds across the discontinuity in grid spacing. Inverting (1.8) and setting the incoming left-characteristic to zero, $\hat{\ell}_1 = 0$, the reflection ratio due to a right moving wave at the interface can be computed

$$\rho = -\frac{R_{-1}}{L_{-1}}\left(\frac{\bar{h}_0 R_{-1}(\bar{h}_1 R_0 - \bar{h}_0 R_1 + \bar{h}_1 L_0) - \bar{h}_1\bar{h}_{-1}R_0 L_0}{\bar{h}_0 L_{-1}(\bar{h}_1 R_0 - \bar{h}_0 R_1 + \bar{h}_1 L_0) - \bar{h}_1\bar{h}_{-1}R_0 L_0}\right),$$

which is nonzero in general.

This is a remarkable example. Although the dispersion relation has no spurious modes, there is a coupling of *physical solution modes* due to grid nonuniformity, and resulting in the reflections visible in Figure 3.1. The box scheme discretization of the wave equation is also included in Figure 3.1 on the right. In this case there are no observable reflections. We provide an explanation in the following section.

4. Box scheme discretization of the wave equation

Similarly, the analysis of §1 can be adapted for the box scheme discretization of (3.1), namely,

$$\frac{\dot{u_j}+\dot{u}_{j+1}}{2}=c\frac{v_{j+1}-v_j}{h_j},\qquad \frac{\dot{v_j}+\dot{v}_{j+1}}{2}=c\frac{u_{j+1}-u_j}{h_j}, \tag{4.1}$$

where again $h_j = x_{j+1} - x_j$.

Applying the time transformation (1.4) to (4.1) gives

$$\frac{-\mathrm{i}\omega}{2}(\hat{u}_{j+1}+\hat{u}_j)=\frac{c}{h_j}(\hat{v}_{j+1}-\hat{v}_j),\qquad \frac{-\mathrm{i}\omega}{2}(\hat{v}_{j+1}+\hat{v}_j)=\frac{c}{h_j}(\hat{u}_{j+1}-\hat{u}_j).$$

These relations yield the recursion

$$\hat{U}_{j+1}=S(\mathrm{i}\omega h_j/c)\hat{U}_j,\quad U_j:=\begin{pmatrix}\hat{u}_j\\ \hat{v}_j\end{pmatrix},\qquad S(z)=\frac{1}{1+(\frac{z}{2})^2}\begin{bmatrix}1-(\frac{z}{2})^2 & z\\ z & 1-(\frac{z}{2})^2\end{bmatrix}, \tag{4.2}$$

and the resulting system is diagonalized

$$S(z)=X(z)D(z)X(z)^{-1},\qquad D(z)=\begin{bmatrix}R(z) & 0\\ 0 & L(z)\end{bmatrix},\qquad X(z)=\begin{bmatrix}-1 & 1\\ 1 & 1\end{bmatrix}. \tag{4.3}$$

where $R(z)$ and $L(z)$ are the eigenvalues of $S(z)$. Specifically,

$$R(z)=\frac{1+\frac{1}{2}z}{1-\frac{1}{2}z},\qquad L(z)=\frac{1-\frac{1}{2}z}{1+\frac{1}{2}z}.$$

For a uniform grid $h \equiv h_j$, $R(\mathrm{i}\omega h_j/c) = \exp(\mathrm{i}\kappa^+ h)$ and $L(\mathrm{i}\omega h_j/c) = \exp(\mathrm{i}\kappa^- h)$ correspond to the positive and negative branches, respectively, of the dispersion relation

$$\omega=\pm\frac{2c}{h}\tan\frac{\kappa h}{2},$$

which is shown in Figure 1.1. Note that $|R(\mathrm{i}\omega h_j/c)| = |L(\mathrm{i}\omega h_j/c| = 1$, i.e. the discretization is nondamping.

Defining characteristic variables $\hat{C}_j = (\hat{r}_j, \hat{\ell}_j)^T$, the recursion (4.2) may be diagonalized:

$$\hat{C}_j := X(\mathrm{i}\omega h_j/c)^{-1}\hat{U}_j,\qquad \hat{C}_{j+1}=D(\mathrm{i}\omega h_j/c)\hat{C}_j \tag{4.4}$$

Again we have both right- and left-moving solutions which evolve independently:

$$\hat{r}_{j+1}=R(\mathrm{i}\omega h_j/c)\hat{r}_j,\qquad \hat{\ell}_{j+1}=L(\mathrm{i}\omega h_j/c)\hat{\ell}_j. \tag{4.5}$$

Note however, that the transformation matrix X is independent of h_j. Consequently, the transformation (4.4) to characteristic variables can be applied globally even on a nonuniform grid. The characteristic families (4.5) decouple on the entire grid, independent of grid spacing. For the grid (1.7) we obtain, across the discontinuity,

$$\hat{r}_1=R_0R_{-1}\hat{r}_{-1},\qquad \hat{\ell}_1=L_0L_{-1}\hat{\ell}_{-1}.$$

In this case, setting the left-characteristic to zero $\hat{\ell}_1 = 0$ leads to $\hat{\ell}_{-1} = 0$ and therefore to $\rho = 0$.

This property (grid independence of X) is not unique to the box scheme, but holds for any Runge-Kutta method, and is a consequence of the fact that RK methods preserve, under discretization, the invariant subspaces of linear ODEs. We discuss this further in the next section.

5. Runge-Kutta spatial discretizations

In this section we consider a general system of N linear, constant coefficient, hyperbolic PDEs

$$u_t + \Phi u_x = 0, \qquad \Phi = Z\Lambda Z^{-1}, \qquad \Lambda = \mathrm{diag}(c_1, \ldots, c_N), \tag{5.1}$$

for $c_n \in \mathrm{R}$. Isolating the spatial derivative in (5.1)

$$u_x = -\Phi^{-1} u_t,$$

we apply an RK method as for an initial value problem to obtain the relation between grid points j and $j+1$. For an s-stage RK method with coefficients a_{ik}, b_i:

$$\begin{array}{l} U_i = -\Phi^{-1}\partial_t(u_j + h_j \sum_{k=1}^{s} a_{ik} U_k), \quad i = 1, \ldots, s \\ u_{j+1} = u_j + h_j \sum_{i=1}^{s} b_i U_i. \end{array} \tag{5.2}$$

Letting $v_j = Z^{-1}u_j$ and $V_k = Z^{-1}U_k$ and pre-multiplying all stages above by Z^{-1} gives

$$\begin{array}{l} V_i = -\Lambda^{-1}\partial_t(v_j + h_j \sum_{k=1}^{s} a_{ik} V_k) \\ v_{j+1} = v_j + h_j \sum_{i=1}^{s} b_i V_i. \end{array}$$

But, since Λ is diagonal, the above formulas decouple. Let $R(z)$ be the stability function (2.4) of the RK scheme. Then, after time-Fourier transformation (1.4), it holds that

$$\hat{v}_{j+1}^n = R(\mathrm{i}\omega h_j / c_n)\hat{v}_j^n, \quad n = 1, \ldots, N \tag{5.3}$$

i.e. the N characteristic families are globally decoupled independent of the mesh. The above recursion is equivalent to applying the RK method in space to the N scalar PDEs

$$\partial_t v^n + c_n \partial_x v^n = 0.$$

That is, discretization followed by diagonalization is equivalent to diagonalization followed by discretization. Note that the matrix of diagonalization is the matrix of eigenvectors of Φ, and is independent of h. We summarize the above discussion in the form of a theorem:

Theorem 5.1 *Let the linear, constant coefficient, system of N hyperbolic PDEs (5.1) be semi-discretized over each interval $[x_j, x_{j+1}]$ by the s-stage Runge-Kutta method (5.2) with coefficients a_{ij}, b_i, $i = 1, \ldots, s$. Then the resulting system of ordinary differential equations decouple into N semi-discrete, scalar recursions (5.3) corresponding to the same discretization applied directly to the characteristic families.*

If, furthermore, the RK method has stability function a diagonal Padé approximation, then the group velocities of the individual modes will have the correct signs, and spurious reflections will not occur.

We note that the above derivation also holds in the case that a different RK method is used in each grid interval. For example, one may use methods of different order in different parts of the domain, i.e. p-refinement can be done without reflections.

As a concrete example of a higher order RK discretization, consider (3.1), and let us apply the symmetric 4th order Lobatto IIIA method (see e.g. [7]), with Butcher array

0	0	0	0
1/2	5/24	1/3	-1/24
1	1/6	2/3	1/6
	1/6	2/3	1/6

Auxiliary variables $U_{j+1/2}$ and $V_{j+1/2}$ are introduced at the half-intervals $x_{j+1/2}$, and the Lobatto method gives the relations

$$\begin{aligned}
U_{j+1/2} &= u_j + hc^{-1}\partial_t(\frac{5}{24}v_j + \frac{1}{3}V_{j+1/2} - \frac{1}{24}v_{j+1}),\\
V_{j+1/2} &= v_j + hc^{-1}\partial_t(\frac{5}{24}u_j + \frac{1}{3}U_{j+1/2} - \frac{1}{24}u_{j+1}),\\
u_{j+1} &= u_j + hc^{-1}\partial_t(\frac{1}{6}v_j + \frac{2}{3}V_{j+1/2} + \frac{1}{6}v_{j+1}),\\
v_{j+1} &= v_j + hc^{-1}\partial_t(\frac{1}{6}u_j + \frac{2}{3}U_{j+1/2} + \frac{1}{6}u_{j+1}).
\end{aligned}$$

These can be further discretized in time, for example by applying the implicit midpoint rule approximation to $\dot{u}_j$, $\dot{v}_j$, $\dot{U}_{j+1/2}$, and $\dot{V}_{j+1/2}$. Doing so results in a linear system for the solution at the new time level. In general, the system above can also be isolated for the time derivatives by introducing suitable boundary conditions, writing down the discretization for all j, and solving a linear system.

The three-point central discretization (3.3) of the second derivative can be written as a one-step method:

$$\begin{aligned}
u_{j+1} &= u_j + hc^{-1}\dot{v}_{j+1},\\
v_{j+1} &= v_j + hc^{-1}\dot{u}_j,
\end{aligned}$$

but in this form falls in the class of partitioned Runge-Kutta (PRK) methods, for which discretization and diagonalization do not commute. The reason for this is clear: the PRK methods rely on a partitioning of the state variables, where the variables in distinct partitions are discretized by different methods. Diagonalization will effect a coupling of partitions, such that diagonalization followed by partitioning will not be equivalent to partitioning followed by diagonalization.

6. Conclusions

We have seen that nonphysical reflections can arise from finite difference discretizations on nonuniform grids, even when the method in question has no spurious solutions to its dispersion relation. Furthermore, we have shown that discretizations which can be written as Runge-Kutta methods with stability function given by a diagonal Padé approximation, are reflection-free.

In general, spurious reflections may also be encountered in problems with varying coefficients, but for which the impedance is uniform. For example, the wave equation

$$u_t = c_1(x)v_x, \quad v_t = c_2(x)u_x$$

has impedance $z(x) = \sqrt{c_1(x)/c_2(x)}$. If we take $c_1(x) \equiv \alpha^2 c_2(x)$, then there should be no reflections at a point of discontinuous jump in coefficients. Also in this case, the Runge-Kutta schemes would give no reflections.

The analysis in this paper is for time-continuous solutions. In general, reflections can also be introduced by a time-integrator if variable step-sizes are used. For example, even with a uniform spatial grid, the staggered spatial discretization (3.2) will develop a nonphysical reflection if staggered time stepping is used and the stepsize is changed abruptly. An RK spatial discretization combined with an RK method in time would be reflection-free.

The Runge-Kutta discretizations of §5 can be applied to nonlinear systems as well. To apply an RK method to nonlinear systems in which the first derivatives cannot be isolated, an approach such as that used for solving implicit differential algebraic equations may be necessary (see e.g. Ch. 4 of [3]). Numerical experiments with nonlinear problems suggest that spurious reflections are absent or at least of much smaller amplitude if Runge-Kutta discretizations are used. This subject is currently under investigation.

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