Energy-conserving semi-discretizations and spurious numerical reflections

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ABSTRACT

We consider energy-conserving semi-discretizations of linear wave equations on nonuniform grids. Specifically we study explicit and implicit skew-adjoint finite difference methods, based on the assumption of an underlying smooth mapping from a uniform grid, applied to the first and second order wave equations. Our interest is in internal reflection of energy at abrupt variations in grid spacing. We show that all node-centered finite difference schemes suffer from reflections. Cell-centered finite difference schemes for the first order wave equation do not have reflections if the numerical dispersion relation is monotone. Runge-Kutta-based spatial semi-discretizations are also considered and these never give reflections. Furthermore, for higher order wave equations, even finite difference schemes with compact stencils and monotone dispersion relations may give reflections due to coupling of physically significant dispersion branches. Again RK schemes avoid this. Finally, we note that all schemes which avoid internal reflections are implicit.

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1. Background

The research reported in this paper grew out of the observation that the box scheme (attributed to Preissman [20] and Keller [15]; cf. Morton [19]), when used to discretize the wave equation on a nonuniform grid, incurs no artificial reflections at abrupt changes in grid spacing, as opposed to some more standard finite difference methods.

The box scheme can be generalized in two ways. First, it can be seen as a cell-centered finite difference method, and so generalized to higher order implicit finite difference schemes. Second, the box scheme can be seen as an application of the implicit midpoint rule, and so generalized to higher order Runge-Kutta methods applied to the spatial derivatives of a system of first order PDEs [21]. The generalization to Runge-Kutta methods is less familiar. However, the use of such methods to solve two-point boundary value problems can be directly generalized to PDEs via the method of lines [2]. Also, such discretizations are related to spectral element methods [7], although here we consider convergence in the limit as the element size tends to zero as opposed to the limit as the approximation order in each element tends to infinity.

Our interest in the box scheme arises from its properties for modelling Hamiltonian wave equations, as proposed by Reich [21] and Bridges & Reich [3]. As such, we will consider only symmetric, non-dissipative methods in this paper. Such discretizations can often be used to semi-discretize Hamiltonian PDEs to yield Hamiltonian ODEs [18] which are suitable for integration by highly stable and conservative symplectic integrators [10, 22, 23]. The results of this paper may also be applicable to nonsymmetric discretizations, however the artificial damping inherent in such

discretizations is particularly strong at high wave numbers, so since artificial reflections tend to be concentrated at the high end of the spectrum, they may be less of an issue for such methods (but the artificial damping may very well be an issue).

In this paper we will consider abrupt (discontinuous) changes in grid spacing. Spurious reflections can often be ameliorated by smoothly varying the grid or by using special interface conditions [4]. However, our interest here is primarily in an absolute property of the methods. Freedom from reflections makes a method more flexible and implies that energy travels in the correct direction.

Deriving finite difference methods that conserve energy on arbitrary grids is challenging. In [16] it is shown that a high order conservative finite difference method that is exact on polynomials on an arbitrary grid must depend globally on the grid. This is certainly impractical. For grids that can be obtained through a smooth mapping $x_j = x(\xi_j)$ from a uniform grid $\xi_j = j\Delta\xi$, high order conservative methods can be constructed by using symmetric discretizations to discretize $\partial u/\partial x = (\partial u/\partial \xi)/(\partial x/\partial \xi)$. For insufficiently smooth $x(\xi)$, loss of order is incurred, and in fact the methods may not even converge. However, for the methods that will be used in this paper, second order is retained for piecewise differentiable $x(\xi)$, as can be shown using a technique of [17]. The Runge-Kutta spatial discretizations are all locally defined on a single grid cell, and being 'unaware' of the surrounding grid, maintain their order on arbitrary grids. These methods can be constructed to arbitrary accuracy.

While we will see that any Runge-Kutta method is reflection-free, only a select class of finite difference schemes is, and these are all implicit.

In the first part of the paper we consider semi-discretizations of the first-order wave or *advection equation*

$$u_t + u_x = 0. \tag{1.1}$$

Assuming $u(x,t), u_t(x,t)$ are L_1 functions of t for all x, (1.1) can be Fourier transformed in time

$$\hat{u}(x,\omega) = \mathcal{F}u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} u(x,t)e^{\mathrm{i}\omega t}\,dt. \tag{1.2}$$

Since $\mathcal{F}u_t = -\mathrm{i}\omega\,\hat{u}$, this yields the complex valued ordinary differential equation

$$\hat{u}_x = \mathrm{i}\omega\hat{u} \tag{1.3}$$

for each frequency ω.

Multiplying both sides of (1.1) by u and integrating yields the energy conservation law

$$\frac{\partial}{\partial t}\left(\frac{u^2}{2}\right) + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = 0,$$

which for appropriate boundary conditions implies the conservation of total energy

$$E = \int \frac{u^2}{2}\,dx. \tag{1.4}$$

The semi-discretizations in this paper conserve a discrete analog of (1.4) on arbitrary grids.

A plane wave $u(x,t) = a\exp\mathrm{i}(\kappa x - \omega t)$ with frequency ω and wave number κ is a nontrivial solution of (1.1) if

$$\omega = \kappa.$$

For a general linear wave equation, the functional relation $\omega(\kappa)$ is referred to as the dispersion relation. A given pulse can be decomposed into a linear combination of plane waves, each propagating with the phase speed ω/κ. The dynamics of the pulse can be interpreted as a mean motion

with the group velocity $d\omega/d\kappa$ plus a dispersion due to mutual differences in phase speed. For (1.1) the phase speed and group velocity are both identically 1, so all pulses translate without dispersing. For numerical discretizations of (1.1), however, this is not so, and the dispersion relation is important for understanding the qualitative behavior of numerical methods [26]. Energy propagates at the group velocity in the sense of Whitham [30].

Many of the issues related to reflections can be expounded in the context of (1.1). However, additional issues arise for higher order derivatives and these can be illustrated for the second order wave equation (henceforth referred to simply as the *wave equation*)

$$u_{tt} - u_{xx} = 0, \tag{1.5}$$

which often arises in applications as a system of first order PDEs

$$u_t = v_x, \qquad v_t = u_x. \tag{1.6}$$

The total energy for the wave equation is

$$E = \int \frac{u^2}{2} + \frac{v^2}{2}\, dx.$$

and its dispersion relation is

$$\omega = \pm\kappa. \tag{1.7}$$

Symmetric methods for (1.1) can be applied directly to the right sides of (1.6), and the properties of the dispersion relation are inherited for each characteristic. However, this approach does not encompass all finite difference equations for (1.6). In particular the popular three-point explicit central difference formula

$$\ddot{u}_j = \frac{1}{h^2}(u_{j-1} - 2u_j + u_{j+1}) \tag{1.8}$$

arises by discretizing (1.6) on a staggered grid. Although this discretization is compact and has a dispersion relation with two monotone branches, the staggering allows a coupling of the characteristics at grid discontinuities that results in artificial internal reflections. This result is far reaching, because staggered schemes are ubiquitous in wave equations. They include some of the *Arakawa grid* discretizations in numerical weather prediction [12], the *Hansen scheme* in computational hydrology [29] and the *Yee scheme* in computational electromagnetics [25]. Furthermore they arise naturally from mimetic discretizations designed to preserve the symmetries of differential operators [24].

2. Finite difference schemes for the advection equation

Let us study the general finite difference method applied to (1.1), see e.g. [13, 14, 5]

$$\sum_{j=0}^{s} \beta_j \dot{u}_{k+j} = -\frac{1}{h}\left(\sum_{j=0}^{s} \alpha_j u_{k+j}\right), \qquad k \in \mathbb{Z}, \tag{2.1}$$

where $h > 0$ is a uniform stepsize and we assume the normalization $\sum_j \beta_j = 1$. If s is even, and $\beta_j = 0$ for $j \neq s/2$, the method is explicit, otherwise it is implicit. We consider symmetric discretizations $\beta_j = \beta_{s-j}$, $\alpha_j = -\alpha_{s-j}$. Furthermore we assume at least one of the pairs (β_0, β_s) or (α_0, α_s) is nonzero. If s is even the discretization is *node-centered*, whereas if s is odd the discretization is *cell-centered*. Cell-centered methods are necessarily implicit.

Define the polynomials

$$\rho(z) = \sum_{j=0}^{s} \alpha_j z^j, \qquad \sigma(z) = \sum_{j=0}^{s} \beta_j z^j$$

and the characteristic function

$$q(z) = \frac{\rho(z)}{\sigma(z)}.$$

In the terminology of [14], the rational function q is termed *good* if if $\sigma(z)$ is nonzero on the unit circle, i.e. $\sigma(e^{\mathrm{i}\kappa}) \neq 0$, $\kappa \in [-\pi, \pi]$. A necessary condition for a semi-discretization (2.1) to be stable is that it be good. We wish to relax this somewhat, since there are semi-discretizations for which $\sigma(-1) = 0$ that are stable when coupled with a suitable implicit time integrator. To that end we exclude the case $\kappa = \pi$ and say (2.1) is good if

$$\sigma(e^{\mathrm{i}\kappa}) \neq 0, \quad \kappa \in (-\pi, \pi).$$

2.1 Monotone dispersion relations

A numerical dispersion relation analogous to (1.7) can be derived for the discretization (2.1) by substituting the semi-discrete plane wave $u_j(t) = \exp \mathrm{i}(\kappa j h - \omega t)$:

$$\omega = \frac{-\mathrm{i}}{h} \frac{\rho(e^{\mathrm{i}\kappa h})}{\sigma(e^{\mathrm{i}\kappa h})}. \tag{2.2}$$

Discretization introduces artificial dispersion, and the phase speed and group velocity are no longer independent of wave number in general. The group velocity is the appropriate quantity in a numerical context, since it determines how numerical perturbations will propagate with respect to the true solution [26].

The analytic dispersion relation (1.7) for the advection equation increases monotonically. We will see that monotonicity is a desirable property for the numerical dispersion relation as well. It can be shown that for symmetric methods, the nonzero roots of ρ and σ satisfy

$$\rho(\lambda) = 0 \Rightarrow \rho(\lambda^{-1}) = 0, \qquad \sigma(\lambda) = 0 \Rightarrow \sigma(\lambda^{-1}) = 0. \tag{2.3}$$

Assume σ is good. By our assumed scaling, $\sigma(1) = 1$ and therefore $\sigma(e^{\mathrm{i}\kappa}) > 0$, for $|\kappa| < \pi$. Then if $\sigma(\lambda) = 0$, either $\lambda = -1$ or the pair λ, λ^{-1}, where $|\lambda| \neq 1$, are both roots of σ. In particular, a cell-centered symmetric finite difference method (with s odd) must have $\sigma(-1) = 0$, since it has an odd number of roots, and for a node-centered symmetric finite difference method, any poles of modulus one must be multiple poles at -1.

Consistency of the discretization (2.1) requires $\rho(1) = 0$, and this cannot be a multiple root. A convergent method must be tangent to the exact dispersion relation at $\kappa = 0$, so $\omega(\kappa)$ is increasing there. If $\rho(e^{\mathrm{i}\kappa^*}) = 0$ for some $\kappa^* \neq 0$, then $\omega(\kappa^*) = 0$, and since $\omega(\kappa)$ is continuous for good methods, the group velocity must change sign on $[0, \kappa^*]$, so the method cannot have a monotone dispersion relation. It follows that if we require monotonicity, then ρ must have precisely one root on the unit circle, and this must be $\rho(1) = 0$, i.e. $\kappa = 0$. All other roots appear in pairs λ, λ^{-1}, where $|\lambda| \neq 1$.

For node-centered discretizations ρ has an even number of roots, $\rho(1) = 0$ is a simple root, so it must hold that $\rho(-1) = 0$. In other words, no node-centered method has a monotone dispersion relation. In particular, no explicit, symmetric finite difference method has a monotone dispersion relation.

It is also clear from the above arguments that for all (irreducible) cell-centered symmetric finite difference methods having monotone dispersion relations, $\omega(\kappa) \to \pm\infty$ at $\kappa = \pm\pi$.

Figure 2.1 displays the dispersion relations for several finite difference methods. On the left are the dispersion relations for node-centered methods: the second order central difference (2.5), the 3-point 4th order scheme defined by $\{\beta_0 = 1/6, \beta_1 = 2/3, \alpha_0 = -1/2\}$, the 5-point 6th order scheme $\{\beta_0 = 1/70, \beta_1 = 8/35, \beta_2 = 18/35, \alpha_0 = -5/84, \alpha_1 = -8/21\}$; and on the right are dispersion relations for edge centered methods: the box scheme (2.10), the 4-point 4th order scheme $\{\beta_0 = -1/16, \beta_1 = 9/16, \alpha_0 = 1/24, \alpha_1 = -27/24\}$, and the 6-point 6th order scheme $\{\beta_0 = 3/256, \beta_1 = -25/256, \beta_2 = 75/128, \alpha_0 = -3/640, \alpha_1 = 25/384, \alpha_2 = -75/64\}$. (The higher order methods lie closer to the analytic dispersion relation.)

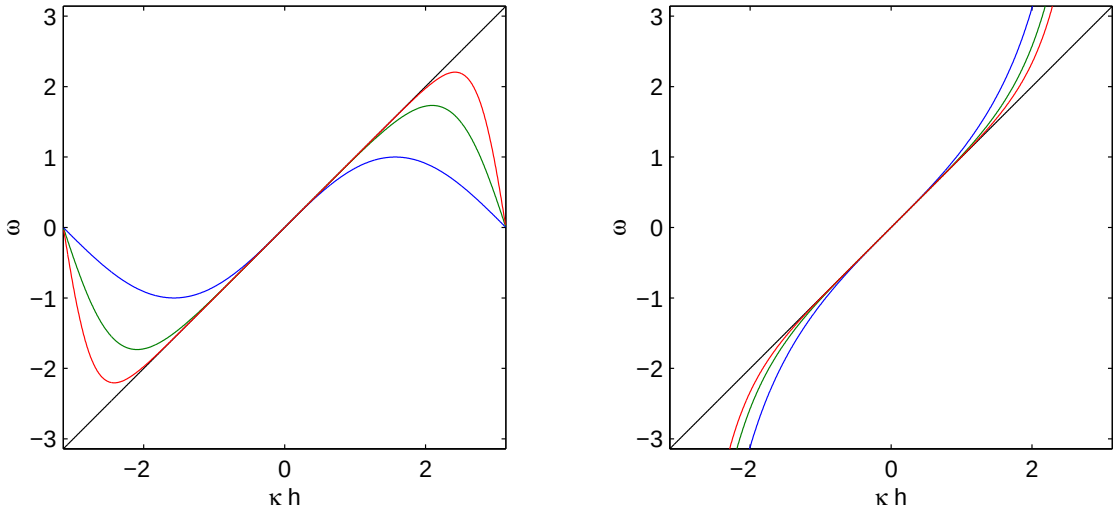

Figure 2.1: Dispersion relations $-\mathrm{i}q(\exp \mathrm{i}\kappa h)$ for (left) node-centered and (right) cell-centered differences. The node-centered schemes are (in increasing order of accuracy) the explicit scheme (2.5) and the 4th and 6th order schemes with $s = 4$ and $s = 6$, respectively. The cell-centered schemes are the box scheme (2.10) and the 4th and 6th order schemes with $s = 3$ and $s = 5$.

2.2 Energy conservation

The class of methods (2.1) with symmetric differences conserves a discrete energy, and when properly implemented, energy conservation can be generalized to nonuniform grids. In [16] this is shown for explicit discretizations. We extend that here to implicit discretizations. To that end, let us assume a periodic domain and introduce circulant matrices E, M and D such that for a grid function $\boldsymbol{u} = (u_j)$,

$$(E\boldsymbol{u})_j = u_{j+1}, \qquad (M\boldsymbol{u})_j = \sum_{k=0}^{s} \beta_k u_{j+k-\lfloor s/2 \rfloor}, \quad (D\boldsymbol{u})_j = \sum_{k=0}^{s} \alpha_k u_{j+k-\lfloor s/2 \rfloor}$$

so that (2.1) can be written in matrix form as

$$M\dot{\boldsymbol{u}} = -h^{-1} D\boldsymbol{u}.$$

Assuming that the mesh satisfies $x_j = x(\xi_j)$, with $dx/d\xi$ bounded away from zero, for a uniform auxiliary mesh $\xi_j = j\Delta\xi$, we discretize the transformed advection equation

$$u_t = -\frac{\partial u/\partial \xi}{\partial x/\partial \xi}$$

by

$$M\dot{\boldsymbol{u}} = -H^{-1} D\boldsymbol{u} \tag{2.4}$$

where $H = \mathrm{diag}(\hat{h}_j)$ and $\hat{h}_j/\Delta\xi \approx \partial x/\partial \xi$ is a consistent approximation at ξ_j for node-centered and $\xi_{j+1/2}$ for cell-centered differences.

The finite difference method (2.4) conserves the discrete energy integral analogous to (1.4)

$$\mathcal{E} = \frac{1}{2}(M\boldsymbol{u})^T H M\boldsymbol{u}.$$

We will show this for the cell-centered case. However, the proof for the node-centered case is identical, but with E replaced by the identity matrix I. The matrices M and D commute:

$MD = DM$ (their eigenvectors are discrete Fourier modes) and satisfy symmetries $M^T = EM$, and $D^T = -ED$. Hence,

$$\dot{\mathcal{E}} = (M\boldsymbol{u})^T HM\dot{\boldsymbol{u}} = -(M\boldsymbol{u})^T D\boldsymbol{u} = -\boldsymbol{u}^T EMD\boldsymbol{u} = -\boldsymbol{u}^T EDM\boldsymbol{u} = (D\boldsymbol{u})^T M\boldsymbol{u} = 0,$$

as desired.

The discretization (2.4) maintains the order of its uniform counterpart (2.1) if the grid mapping $x(\xi)$ is sufficiently smooth and $dx/d\xi > 0$ is bounded above and below by positive constants. For arbitrary grids, the accuracy is reduced and indeed the method need not converge.

2.3 Reflections: an example

In [28, 27] Vichnevetsky gives an analysis of the reflections observed when the 2nd order explicit central difference method

$$\dot{u}_j = -\frac{u_{j+1} - u_{j-1}}{x_{j+1} - x_{j-1}}, \tag{2.5}$$

($s = 2$, $\beta = [\ 0 \quad 1 \quad 0\ ]$, $\alpha = [\ -1/2 \quad 0 \quad 1/2\ ]$) is applied on a piecewise uniform grid with an abrupt change in grid spacing

$$x_j = \begin{cases} jh^+, & j \geq 0 \\ jh^-, & j < 0 \end{cases} \tag{2.6}$$

where $h^+ \neq h^-$.

Since (2.5) is an explicit finite difference method, its dispersion relation cannot be monotone. In fact (2.2) has two solutions κ^+ and κ^- for each $\omega h \in (-1, 1)$ (see Figure 2.1). These are the two solutions of

$$\omega = \frac{1}{h} \sin \kappa h.$$

The group velocities $\omega'(\kappa^\pm) = \cos \kappa^\pm h$ have opposite signs, and we identify κ^+ with the mode having positive group velocity $|\kappa^+| < \pi/2$ and κ^- with the negative one $|\kappa^-| > \pi/2$.

Applying the time transformation (1.2) to (2.5) gives the difference equation

$$\hat{u}_{j+1} - \mathrm{i}2\omega\bar{h}_j\hat{u}_j - \hat{u}_{j-1} = 0 \tag{2.7}$$

where $\bar{h}_j \equiv \frac{1}{2}(x_{j+1} - x_{j-1})$. This recursion is written as a one-step method

$$\hat{\boldsymbol{U}}_{j+1} = S_j\hat{\boldsymbol{U}}_j, \qquad \hat{\boldsymbol{U}}_j = \begin{pmatrix} \hat{u}_j \\ \hat{u}_{j-1} \end{pmatrix}, \qquad S_j = \begin{bmatrix} \mathrm{i}2\omega\bar{h}_j & 1 \\ 1 & 0 \end{bmatrix} \tag{2.8}$$

The matrix S_j can be decomposed as

$$S_j = X_j D_j X_j^{-1}, \qquad D_j = \begin{bmatrix} \lambda_j^+ & \\ & \lambda_j^- \end{bmatrix}, \qquad X_j = \begin{bmatrix} \lambda_j^+ & \lambda_j^- \\ 1 & 1 \end{bmatrix},$$

where λ_j^+ and λ_j^-, the eigenvalues of S_j, are the roots of the characteristic polynomial associated with (2.7)

$$\lambda_j^+ = \mathrm{i}\omega\bar{h}_j + \sqrt{1 - \omega^2\bar{h}_j^2}, \qquad \lambda_j^- = \mathrm{i}\omega\bar{h}_j - \sqrt{1 - \omega^2\bar{h}_j^2}$$

For $|\omega\bar{h}_j| < 1$, the eigenvalues have modulus one, and can be related to the two wave numbers κ^+ and κ^- for the given value of $\omega\bar{h}_j$ in the dispersion relation (2.2). Specifically:

$$R_j := \lambda_j^+ = e^{\mathrm{i}\kappa^+\bar{h}_j}, \qquad L_j := \lambda_j^- = e^{\mathrm{i}\kappa^-\bar{h}_j}$$

Introducing characteristic variables

$$\hat{\boldsymbol{C}}_j = X_j^{-1}\hat{\boldsymbol{U}}_j = \begin{pmatrix} \hat{r}_j \\ \hat{\ell}_j \end{pmatrix},$$

the recursion (2.8) transforms to give

$$\hat{\boldsymbol{C}}_{j+1} = X_{j+1}^{-1} X_j D_j \hat{\boldsymbol{C}}_j.$$

On a uniform grid $\bar{h}_j \equiv h$, we have $X_{j+1} = X_j$, yielding

$$\hat{r}_{j+1} = R_j \hat{r}_j, \qquad \hat{\ell}_{j+1} = L_j \hat{\ell}_j.$$

That is, there are left and right moving solutions, which are decoupled on a uniform grid.

On the grid (2.6), $\bar{h}_{-1} \neq \bar{h}_0 \neq \bar{h}_{-1}$, and the characteristic solutions do not decouple there. Across the discontinuity we have

$$\hat{\boldsymbol{C}}_1 = X_1^{-1} X_0 D_0 X_0^{-1} X_{-1} D_{-1} \hat{\boldsymbol{C}}_{-1}.$$

Now, suppose there is a wave incident from the left, so $\hat{r}_{-1}$ is nonzero, and there is no incident wave from the right, so $\hat{\ell}_1 = 0$ (away from x_0, the grid is uniform and the left and right characteristics are decoupled). Then from the above equality the ratio of reflected to incident wave amplitudes in $\mathbb{R}^-$ can be computed

$$\frac{\hat{\ell}_{-1}}{\hat{r}_{-1}} = -\frac{R_{-1}}{L_{-1}} \left(\frac{R_{-1}(R_0 - R_1 + L_0) - R_0 L_0}{L_{-1}(R_0 - R_1 + L_0) - R_0 L_0} \right),$$

and will be nonzero, in general.

The effect of grid nonuniformity is an exchange of energy between fundamental solution modes. This result can be generalized to all finite difference methods with nonmonotone dispersion relations.

2.4 Reflections: the general case

We consider the difference formula (2.1), applied on a nonuniform grid (i.e. with h replaced by $\hat{h}_j$ as in (2.4).)

Introducing the vector $\hat{\boldsymbol{U}}_j = (\hat{u}_{j+s-1}, \hat{u}_{j+s-2}, \ldots, \hat{u}_j)^T$ we can write (2.1) as a one-step method

$$\hat{\boldsymbol{U}}_{j+1} = S_j(\omega)\hat{\boldsymbol{U}}_j \tag{2.9}$$

where the matrix $S_j(\omega)$ has the structure

$$S_j(\omega) = \begin{pmatrix} \mu_{s-1}^j & \mu_{s-2}^j & \cdots & \mu_1^j & a_0^j \\ 1 & 0 & & & \\ & 1 & 0 & & \\ & & \ddots & & \\ & & & 1 & 0 \end{pmatrix}, \qquad \mu_k^j = -\frac{\alpha_k - \mathrm{i}\omega\hat{h}_j\beta_k}{\alpha_s - \mathrm{i}\omega\hat{h}_j\beta_s}.$$

Denote the eigenvalues of S_j by $\lambda_{j,k}$, $k = 1, \ldots, s$, and suppose these are distinct.[1] Furthermore, assume that two eigenvalues have modulus 1, corresponding to group velocites with opposite sign: $\lambda_{j,1} = e^{\mathrm{i}\kappa_1\hat{h}_j} =: R_j$ and $\lambda_{j,2} = e^{\mathrm{i}\kappa_2\hat{h}_j} =: L_j$.

[1] This assumption could be relaxed to requiring distinction among eigenvalues of unit modulus, which is certainly the case if we are considering multiple solutions of a nonmonotone dispersion relation.

Since the eigenvalues are distinct, S_j can be written as

$$S_j = X_j D_j X_j^{-1},$$

where $D_j = \mathrm{diag}(\lambda_{j,1}, \lambda_{j,2}, \ldots, \lambda_{j,s})$ and it is easy to see that X_j is the Vandermonde matrix

$$X_j = \begin{pmatrix} \lambda_{j,1}^{s-1} & \lambda_{j,2}^{s-1} & \cdots & \lambda_{j,2}^{s-1} \\ \vdots & \vdots & \vdots & \vdots \\ \lambda_{j,1} & \lambda_{j,2} & \cdots & \lambda_{j,2} \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

Let $\hat{\boldsymbol{Z}}_j = X_j^{-1}\hat{\boldsymbol{U}}_j$, $\hat{\boldsymbol{Z}}_j = (\hat{r}_j, \hat{\ell}_j, \hat{z}_{j,3}, \cdots, \hat{z}_{j,s})^T$. Then (2.9) can be written

$$\hat{\boldsymbol{Z}}_{j+1} = X_{j+1}^{-1} X_j D_j \hat{\boldsymbol{Z}}_j$$

Denoting $B = (b_{mn}) = X_{j+1}^{-1} X_j$, we have

$$\begin{aligned} \hat{r}_{j+1} &= b_{11} R_j \hat{r}_j + b_{12} L_j \hat{\ell}_j + b_{13} \lambda_{j,3} \hat{z}_{j,3} + \cdots \\ \hat{\ell}_{j+1} &= b_{21} R_j \hat{r}_j + b_{22} L_j \hat{\ell}_j + b_{23} \lambda_{j,3} \hat{z}_{j,3} + \cdots \\ \hat{z}_{j+1,3} &= b_{31} R_j \hat{r}_j + b_{32} L_j \hat{\ell}_j + b_{33} \lambda_{j,3} \hat{z}_{j,3} + \cdots \\ &\vdots \end{aligned}$$

If $X_{j+1} = X_j$, for example where the grid is uniform, these relations reduce to

$$\begin{aligned} \hat{r}_{j+1} &= R_j \hat{r}_j \\ \hat{\ell}_{j+1} &= L_j \hat{\ell}_j \\ \hat{z}_{j+1,3} &= \lambda_{j,3} \hat{z}_{j,3} \\ &\vdots \end{aligned}$$

and the fundamental modes are decoupled.

In general, however, the modes will be coupled. To avoid an exchange of energy between modes 1 and 2 we need $b_{12} = b_{21} = 0$. This is equivalent to

$$\begin{aligned} b_{12} &= \boldsymbol{e}_1^T X_{j+1}^{-1} X_j \boldsymbol{e}_2 = (X_{j+1}^{-T} \boldsymbol{e}_1)^T X_j \boldsymbol{e}_2 = 0, \\ b_{21} &= \boldsymbol{e}_2^T X_{j+1}^{-1} X_j \boldsymbol{e}_1 = (X_{j+1}^{-T} \boldsymbol{e}_2)^T X_j \boldsymbol{e}_1 = 0, \end{aligned}$$

where $\boldsymbol{e}_k$ denotes the kth canonical unit vector in $\mathbb{R}^s$. Now, since X_{j+1} is a Vandermonde matrix, the vectors $X_{j+1}^{-T}\boldsymbol{e}_1$ and $X_{j+1}^{-T}\boldsymbol{e}_2$ are simply the coefficients of the Lagrange interpolating polynomials $p_1(x)$ and $p_2(x)$ for the eigenvalues $\lambda_{j,k}$, i.e.

$$p_1(x) = \frac{x - L_{j+1}}{R_{j+1} - L_{j+1}} \prod_{k=3}^{s} \frac{x - \lambda_{j+1,k}}{R_{j+1} - \lambda_{j+1,k}}, \qquad p_2(x) = \frac{x - R_{j+1}}{L_{j+1} - R_{j+1}} \prod_{k=3}^{s} \frac{x - \lambda_{j+1,k}}{L_{j+1} - \lambda_{j+1,k}}.$$

Furthermore, since $X_j \boldsymbol{e}_2 = (L_j^{s-1}, \cdots L_j, 1)^T$ and $X_j \boldsymbol{e}_1 = (R_j^{s-1}, \cdots R_j, 1)^T$, it follows that to avoid an exchange of energy between modes 1 and 2,

$$b_{12} = p_1(L_j) = 0, \qquad b_{12} = p_2(R_j) = 0.$$

Assuming S_j has only two eigenvalues of modulus 1, we conclude that

$$L_j = L_{j+1}, \qquad R_j = R_{j+1}$$

is necessary to avoid reflections. However this implies the grid must be uniform.

This result can be easily generalized to $k > 2$ eigenvalues of modulus one.

Proposition 1 *If the dispersion relation (2.2) of finite difference method (2.1) is nonmonotone, then there will be an exchange of energy between oscillatory modes at a grid nonuniformity.*

If the dispersion relation is monotone, then (2.2) has a unique real solution κ for each ω. There may also be complex solutions, and these will correspond to exponentially growing and decaying modes. Such modes must be constrained by boundary conditions.

The simplest example of a finite difference method with monotone dispersion relation is the box scheme:

$$\frac{1}{2}(\dot{u}_{j+1} + \dot{u}) = -\frac{1}{h}(u_{j+1} - u_j), \tag{2.10}$$

for which

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

As a one-step method, the box scheme has one real and no complex solutions to the dispersion relation.

In the next section we consider a different generalization of the box scheme, as a Runge-Kutta method.

3. Runge-Kutta semi-discretizations for the advection equation

It is straightforward to apply a Runge-Kutta method to the spatial derivative of the advection equation [21] (see also [6]. This is analogous to what is done for boundary value problems [2]. We write

$$u_x = -u_t,$$

and apply the RK method as for an initial value problem in x to obtain the relation between grid points j and $j+1$. For an s-stage RK method with coefficient matrices (see [9]) $A \in \mathbb{R}^{s\times s}$ and $\boldsymbol{b} \in \mathbb{R}^s$ and stage vectors $\boldsymbol{U}_j \in \mathbb{R}^s$:

$$\begin{aligned} \boldsymbol{U}_j &= \mathbb{1}u_j - h_j A\partial_t \boldsymbol{U}_j, \\ u_{j+1} &= u_j - h_j \boldsymbol{b}^T \partial_t \boldsymbol{U}_j \end{aligned} \tag{3.1}$$

where $\mathbb{1} = (1,\ldots,1)^T \in \mathbb{R}^s$ and $h_j := x_{j+1} - x_j$.

To analyze the stability of this process, we assume an infinite domain, uniform grid spacing h, and that $\sum_j |u_j|^2 < \infty$. Then we apply the semi-discrete Fourier transform to (3.1)

$$\hat{u}(t,\kappa) = \sum_j u_j(t)e^{-\mathrm{i}j\kappa h}, \quad \hat{\boldsymbol{U}}(t,\kappa) = \sum_j \boldsymbol{U}_j(t)e^{-\mathrm{i}j\kappa h},$$

(i.e. multiplying both sides of each equation with $\exp(-\mathrm{i}j\kappa h)$ and summing over all j), where κ is a wavelength such that $\kappa h \in [-\pi,\pi]$. For the second equation above, this yields

$$(e^{\mathrm{i}\kappa h} - 1)\hat{u} = -h\boldsymbol{b}^T\partial_t\hat{\boldsymbol{U}},$$

which, when substituted into the transformed first equation, gives

$$(e^{\mathrm{i}\kappa h} - 1)\hat{\boldsymbol{U}} = -h\mathbb{1}\boldsymbol{b}^T\partial_t\hat{\boldsymbol{U}} - h_j(e^{\mathrm{i}\kappa h} - 1)A\partial_t\hat{\boldsymbol{U}},$$

i.e.,

$$-h\left[\mathbb{1}\boldsymbol{b}^T - (e^{\mathrm{i}\kappa h} - 1)A\right]\partial_t\hat{\boldsymbol{U}}_j = (e^{\mathrm{i}\kappa h} - 1)\hat{\boldsymbol{U}} \tag{3.2}$$

For stability we therefore require that for z a generalized eigenvalue satisfying

$$\det\left(z\left[\mathbb{1}\boldsymbol{b}^T + (e^{\mathrm{i}\kappa h} - 1)A\right] - (e^{\mathrm{i}\kappa h} - 1)I\right) = 0,$$

we have $z \in \mathbb{C}^+$, the nonnegative half-plane.

Define the *stability function* of the RK method [9]:

$$R(z) = 1 + z\boldsymbol{b}^T(I - zA)^{-1}\mathbb{1}.$$

This function is a rational function whose finite poles are the set $\mathcal{P} = \{z \in \mathbb{C}; \det(I - zA) = 0\}$. Denote by $G(z)$ the matrix

$$G(z) = I + z(I - zA)^{-1}\mathbb{1}\boldsymbol{b}^T.$$

Since $R(z)\boldsymbol{b}^T = \boldsymbol{b}^T G(z)$, it follows that $R(z)$ is an eigenvalue of $G(z)$ associated with left eigenvector $\boldsymbol{b}$. Therefore, it holds that

$$\det(G(z) - R(z)I) = 0.$$

The stability domain is defined as $\mathcal{S} = \{z \in \mathbb{C}; |R(z)| \leq 1\}$. The boundary of this domain $\partial\mathcal{S}$ is characterized by the set of z such that $R(z) = \exp(\mathrm{i}\theta)$ for $\theta \in (-\pi, \pi]$. For $z \in \partial\mathcal{S}$ we have

$$\begin{aligned} 0 &= \det(G(z) - e^{\mathrm{i}\theta}I) \\ &= \det((1 - e^{\mathrm{i}\theta})I + z(I - zA)^{-1}\mathbb{1}b^T) \\ &= \det(I - zA)^{-1}\det(z(e^{\mathrm{i}\theta} - 1)A + z\mathbb{1}b^T - (e^{\mathrm{i}\theta} - 1)I). \end{aligned}$$

Values of z making the first determinant zero are precisely the poles of the stability function R, so clearly they are not on the boundary of the stability region. Therefore it must be so that the second determinant is zero. However, this is precisely the condition for z to be a generalized eigenvalue of (3.2). Stability of the Runge-Kutta discretization is therefore implied by the condition that $\partial\mathcal{S} \subset \mathbb{C}^+$. Such is the case for A-stable RK methods. Note that if an RK method has a stability boundary entirely in the left half-plane, its adjoint method has a stability boundary entirely in the right half-plane and vice-versa. This is related to the stability of upwind and downwind methods. However, a method whose stability domain contains a subset of the imaginary axis in its interior will be unstable, as will its adjoint. [2]

For symmetric RK methods, $|R(iy)| = 1$. If A has only positive eigenvalues, $\mathcal{P} \subset \mathbb{C}^+$, R is analytic on $\mathbb{C}^-$, and the maximum principle gives A-stability. If R does have poles in $\mathbb{C}^-$ (the nonpositive half-plane), the symmetric RK method is an unstable spatial discretization for advection.

For systems such as the second order wave equation (1.6) where both left and right characteristics are present, stability thus demands the use of symmetric RK methods. Furthermore, for hyperbolic problems where the flow direction may change sign locally, stability of nonsymmetric RK methods requires choosing either a method or its adjoint locally according to the flow direction (i.e. upwinding).

Substituting the plane wave solution $u_j(t) = \exp\mathrm{i}(\kappa hj - \omega t)$ into (3.1) yields the numerical dispersion relation

$$e^{\mathrm{i}\kappa h} = R(\mathrm{i}\omega h). \tag{3.3}$$

Lemma 1 of Guglielmi & Hairer [8] implies that if a symmetric RK method is A-stable, then κ increases monotonically with ω, i.e. the dispersion relation is monotone [6].

Furthermore, it clear from (3.3) that to each ωh there corresponds a unique $\kappa h \in [-\pi, \pi]$, i.e. there is only one mode, and exchange of energy between modes is impossible:

[2] For multistep methods and related finite difference discretizations for advection, a similar relationship between the stability domain of a time integrator and stability of the spatial discretization holds. This fact is implicit in a number of books, for example, [14, 13]. For example, this implies that the BDF formulas of order higher than 2 are unstable spatial discretizations for advection.

Proposition 2 *If (1.1) is discretized using an A-stable symmetric Runge-Kutta method (3.1), then there are no reflections due to nonuniformity of the grid.*

Remark. In fact, when the advection equation (1.1) is equipped with a boundary condition $u(0,t) = g(t)$ on the left side of a domain of finite length L, the RK discretization (3.1) is exactly nonreflecting at the right boundary, with no need of a supplementary numerical boundary condition.

Remark. Lemma 1 of [8] requires the stability region to be connected, which may fail if the symmetric RK method has poles in the left half-plane. Indeed, a counter-example is given by the following two-parameter class of methods

$$A = \begin{bmatrix} \alpha & \beta \\ 1/2-\beta & 1/2-\alpha \end{bmatrix}, \quad b = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}. \tag{3.4}$$

These methods are symmetric and at least second order accurate. The stability domain includes the imaginary axis for any choice of (α, β), and thus is *unconditionally stable* as a numerical integrator for purely oscillatory linear ODEs. For $\gamma \equiv (\alpha-\beta)[1-(\alpha+\beta)] > 0$, the method is additionally A-stable, provides a stable discretization of the advection equation and a monotone dispersion relation. For $\gamma < 0$, however, there is a pole in the left half-plane. The method is no longer A-stable, has a non-monotone dispersion relation, and is an unstable discretization of advection. The stability domain for the case $\alpha = 1/8$, $\beta = 1/4$ is plotted in Figure 3.1.

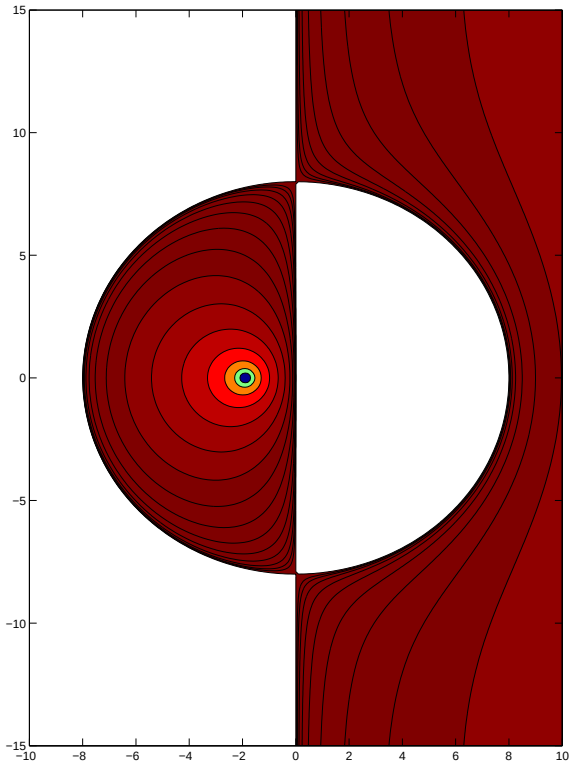

Figure 3.1: Stability domain $\mathcal{S}$ for (3.4).

4. Additional considerations for the wave equation

Higher order wave equations add extra complexity to the picture because the dispersion relation has multiple branches. Even a compact finite difference scheme, with no spurious roots and

monotone branches, can exhibit reflections on a nonuniform grid due to coupling of the branches. We illustrate this for the wave equation (1.5).

A finite difference method in the form (2.4) can be directly applied to the wave equation in first order form (1.6):

$$M\dot{\boldsymbol{u}} = H^{-1}D\boldsymbol{v}, \qquad M\dot{\boldsymbol{v}} = H^{-1}D\boldsymbol{u}.$$

Defining $\boldsymbol{r} = \boldsymbol{u} - \boldsymbol{v}$ and $\boldsymbol{\ell} = \boldsymbol{u} + \boldsymbol{v}$, and taking the sum and difference of the above equations yields

$$M\dot{\boldsymbol{r}} = -H^{-1}D\boldsymbol{r}, \qquad M\dot{\boldsymbol{\ell}} = H^{-1}D\boldsymbol{\ell}, \tag{4.1}$$

and we see that the solution can be decomposed into right and left characteristics, each satisfying an advection equation under the original discretization. In this case, the properties of the advection discretization are directly inherited. Reflections will occur if the numerical dispersion relation is nonmonotone.

However the above approach does not account for all finite difference approximations to the second order wave equation (1.5). For example, the 3-point second order central discretization (1.8) arises through discretization of (1.6) on a staggered grid. Introducing gridpoints at the half-steps $x_{j+1/2} = (x_j + x_{j+1})/2$, let $u_j \approx u(x_j)$ and $v_{j+1/2} \approx v(x_{j+1/2})$. Define the staggered central discretization

$$\dot{u}_j = \frac{1}{\bar{h}_j}(v_{j+1/2} - v_{j-1/2}), \qquad \dot{v}_{j+1/2} = \frac{1}{h_j}(u_{j+1} - u_j), \tag{4.2}$$

where $h_j = x_{j+1} - x_j$ and $\bar{h}_j = (x_{j+1} - x_{j-1})/2$. On a uniform grid, $h \equiv h_j \equiv \bar{h}_j$, this discretization reduces to (1.8). The numerical dispersion relation,

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

is shown on the left in Figure 4.1. It has two branches, corresponding to the right and left characteristics, and each branch is monotone. The dispersion relation has no spurious roots.

Yet, as illustrated on the right of the figure, a numerical simulation of a right-moving pulse, computed using (4.2) on a grid (2.6) with $h^-/h^+ = 7$, clearly incurs reflections at the interface x_0.

The analysis of [28, 27] can be adapted to study this case. Applying the Fourier transformation (1.2) to (4.2), let $\hat{\boldsymbol{U}}_j := (\hat{u}_j, \hat{v}_{j-1/2})^T$. This yields a grid recursion

$$\hat{\boldsymbol{U}}_{j+1} = S_j\hat{\boldsymbol{U}}_j, \qquad S_j = \begin{bmatrix} 1 - \omega^2 h_j\bar{h}_j & -\mathrm{i}\omega h_j \\ -\mathrm{i}\omega\bar{h}_j & 1 \end{bmatrix}. \tag{4.3}$$

The roots of S_j define the numerical dispersion relation, and using group velocity, the roots are identified with the right and left branches:

$$e^{\mathrm{i}\kappa^+ h} = R_j = 1 - \frac{1}{2}\omega^2 h_j\bar{h}_j + \mathrm{i}\sqrt{\omega^2 h_j\bar{h}_j - \frac{1}{4}\omega^4 h_j^2\bar{h}_j^2},$$
$$e^{\mathrm{i}\kappa^- h} = L_j = 1 - \frac{1}{2}\omega^2 h_j\bar{h}_j - \mathrm{i}\sqrt{\omega^2 h_j\bar{h}_j - \frac{1}{4}\omega^4 h_j^2\bar{h}_j^2},.$$

We diagonalize S_j (assuming $\omega^2 h_j\bar{h}_j < 4$)

$$S_j = X_j D_j X_j^{-1}, \qquad D_j = \begin{bmatrix} R_j & \\ & L_j \end{bmatrix} \qquad X_j = \begin{bmatrix} \frac{\mathrm{i}}{\omega\bar{h}_j}R_j & \frac{\mathrm{i}}{\omega\bar{h}_j}L_j \\ 1 & 1 \end{bmatrix}.$$

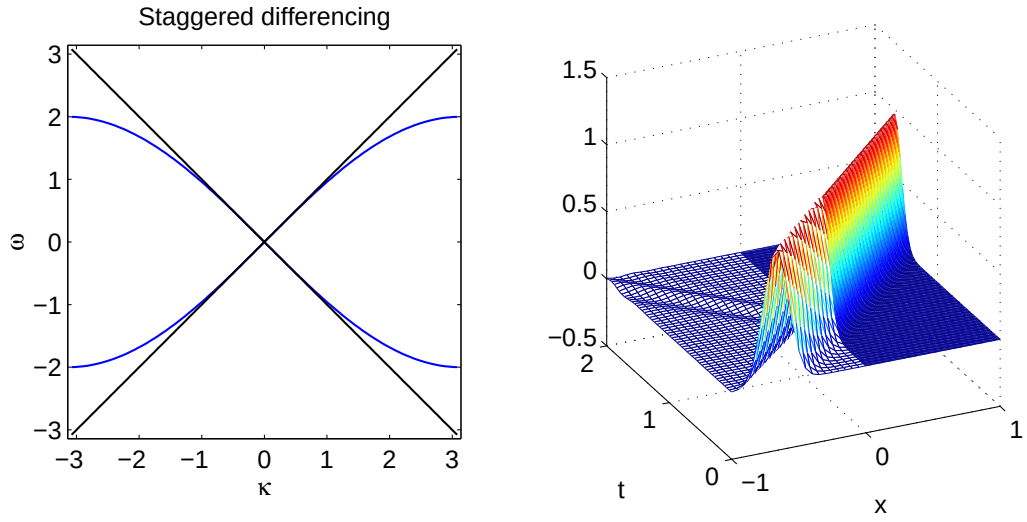

Figure 4.1: The dispersion relation (left, in blue) of the second order staggered differencing scheme (4.2). On the right is a space-time plot of the solution of a traveling pulse computed with this scheme on a grid (2.6) and showing a reflection.

Define characteristic variables $\hat{\boldsymbol{C}}_j := X_j^{-1}\hat{\boldsymbol{U}}_j$ where $\hat{\boldsymbol{C}}_j = (\hat{r}_j, \hat{\ell}_j)^T$. On a uniform grid, X_j is constant independent of j and the recursion (4.3) simplifies to $\hat{\boldsymbol{C}}_{j+1} = D_j\hat{\boldsymbol{C}}_j$. The relations $\hat{r}_{j+1} = R_j\hat{r}_j$, $\hat{\ell}_{j+1} = L_j\hat{\ell}_j$ hold, i.e. the characteristics are decoupled.

Next consider the grid (2.6). Away from x_0 the grid is uniform and the characteristics are decoupled as above. However, across the grid discontinuity, the recursion

$$\hat{\boldsymbol{C}}_1 = X_1^{-1}X_0D_0X_0^{-1}X_{-1}D_{-1}\hat{\boldsymbol{C}}_{-1}, \tag{4.4}$$

holds. If we assume there is a right-moving wave in $\{x < 0\}$ and no left-moving wave in $\{x \geq 0\}$, i.e. set $\hat{\ell}_1 = 0$, then we may solve (4.4) for the reflection ratio $\hat{\ell}_{-1}/\hat{r}_{-1}$, to give

$$\frac{\hat{\ell}_{-1}}{\hat{r}_{-1}} = -\frac{R_{-1}}{L_{-1}}\left(\frac{\bar{h}_0R_{-1}(\bar{h}_1R_0 - \bar{h}_0R_1 + \bar{h}_1L_0) - \bar{h}_1\bar{h}_{-1}R_0L_0}{\bar{h}_0L_{-1}(\bar{h}_1R_0 - \bar{h}_0R_1 + \bar{h}_1L_0) - \bar{h}_1\bar{h}_{-1}R_0L_0}\right),$$

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

To apply a Runge-Kutta semi-discretization as suggested in [21], a higher order PDE is first written in first order form. For the wave equation, the RK method (3.1) is applied uniformly to the spatial derivatives of (1.6).

$$\begin{aligned}
\boldsymbol{V}_j &= \mathbb{1}v_j + h_jA\partial_t\boldsymbol{U}_j, \qquad & v_{j+1} &= v_j + h_j\boldsymbol{b}^T\partial_t\boldsymbol{U}_j,\\
\boldsymbol{U}_j &= \mathbb{1}u_j + h_jA\partial_t\boldsymbol{V}_j, \qquad & u_{j+1} &= u_j + h_j\boldsymbol{b}^T\partial_t\boldsymbol{V}_j.
\end{aligned}$$

Defining $L_j = U_j + V_j$, $R_j = U_j - V_j$, $\ell_j = u_j + v_j$, and $r_j = u_j - \ell_j$, and taking sums and

differences in the above relations gives

$$\boldsymbol{L}_j = \mathbb{1}\ell_j + h_j A\partial_t \boldsymbol{L}_j, \qquad \ell_{j+1} = \ell_j + h_j \boldsymbol{b}^T \partial_t \boldsymbol{L}_j,$$
$$\boldsymbol{R}_j = \mathbb{1}r_j - h_j A\partial_t \boldsymbol{R}_j, \qquad r_{j+1} = r_j - h_j \boldsymbol{b}^T \partial_t \boldsymbol{R}_j.$$

The semi-discrete system is thus decoupled into left and right characteristic advection equations and the analysis of §3 applies. Specifically, there can be no reflections.

On the other hand, if distinct RK methods are used to discretize each of (1.6), reflections could be generated. In particular, the discretization (1.8) can be derived as a *partitioned* RK method applied to (1.6).

We conclude, first, that the reflections can occur due to staggering, even when the dispersion relation has no spurious branches and is monotone, and second, that also for higher order derivatives, explicit finite difference methods are plagued by reflections.

5. Numerical Experiments

In this section we illustrate the ideas of the paper with numerical experiments. In all experiments we solve the wave equation (1.6).

5.1 Reflections in explicit finite difference methods

We solve the wave equation (1.6) using the fourth order, explicit, staggered central finite difference method

$$\dot{u}_i = \frac{2}{x_{i+1/2} - x_{i-1/2}}\left(\frac{1}{24}v_{i-3/2} - \frac{27}{24}v_{i-1/2} + \frac{27}{24}v_{i+1/2} - \frac{1}{24}v_{i+3/2}\right)$$
$$\dot{v}_{i+1/2} = \frac{2}{x_{i+1} - x_i}\left(\frac{1}{24}u_{i-1} - \frac{27}{24}u_i + \frac{27}{24}u_{i+1} - \frac{1}{24}u_{i+2}\right).$$

For smooth grid functions $x(\xi)$, this discretization retains fourth order accuracy. For the grid (2.6) the accuracy is reduced to second order. The domain is $[-2, 2]$ with periodic boundary conditions. We take $h^+/h^- = 7$ by choosing a grid of dimension N and placing $N/8$ of the grid points to the left of the origin and $7N/8$ of the grid points to the right of the origin. The initial conditions are given by

$$u(x,0) = \exp\left(-\frac{30^2}{L^2}(x - \frac{2}{3})^2\right), \qquad v(x,0) = -u(x,0)$$

and define a Gaussian pulse that travels with unit speed to the right. The discrete equations were integrating using the classical fourth order explicit Runge-Kutta scheme with stepsize $\Delta t = (2N)^{-1}$.

The error in the numerical solution as a function of x and t is shown in Figure 5.1 for $N = 200$, 400, and 800.

It is remarkable that although the error in the transmitted wave converges with fourth order accuracy, the spurious reflected wave converges at only second order.

5.2 Absence of reflections with Runge-Kutta box schemes

We solve the same problem as in the previous subsection using a sixth order Gauss-Legendre Runge-Kutta method (3.1) with coefficients

$$A = \begin{bmatrix} \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\ \frac{5}{36} - \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} + \frac{\sqrt{15}}{24} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \end{bmatrix}, \quad \boldsymbol{b} = \begin{pmatrix} \frac{5}{18} \\ \frac{4}{9} \\ \frac{5}{18} \end{pmatrix}$$

A grid of dimension $N = 801$ is used, and time integration is done with stepsize $\Delta t = 1/1600$, using the second order implicit midpoint rule. The error is shown in Figure 5.2. No reflection is observable.

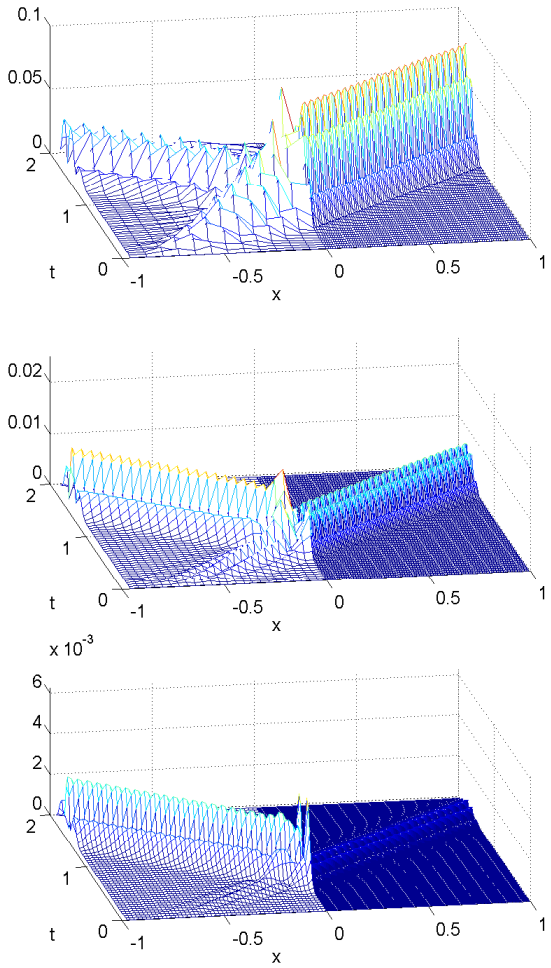

Figure 5.1: Error as a function of space and time for (1.6) computed using a staggered fourth order central scheme on a grid with abrupt change in spacing, for $N = 200$ (top), $N = 400$ (middle) and $N = 800$ (bottom).

5.3 Nonreflecting boundary conditions

Finally, we compute the solution to the wave equation on [0,1] with boundary conditions $r = u - v = 0$ at $x = 0$ and $\ell = u + v = 0$ at $x = 1$, which are exactly nonreflecting boundary conditions for the wave equation.

We discretize (1.6) using the box scheme (2.10) on a uniform grid with $N = 100$ and $\Delta t = 1/100$ on $t \in [0, 1]$.

The boundary conditions are simply

$$u_0 = v_0, \qquad u_N = -v_N.$$

The initial condition is

$$u(x, 0) = \exp(-15^2(x - \frac{1}{2})^2), \qquad v(x, 0) = 0,$$

which splits into left and right going pulses.

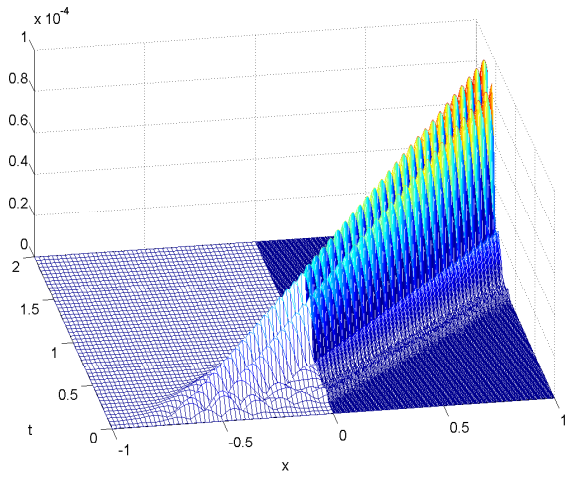

Figure 5.2: Error as a function of space and time for (1.6 computed with a sixth order Gauss-Legendre Runge-Kutta spatial discretization, on a discontinuous grid with $N = 800$.

Figure 5.3 shows a density plot of $\log_{10} u$ as a function of space and time. All noise at machine precision was rounded to 10^{-14}. Clearly, no wave is reflected back as the pulses exit the domain. Of course, this result is special to the wave equation, for which the nonreflecting boundary condition is local, and to a single spatial dimension, for which the angle of incidence is known.

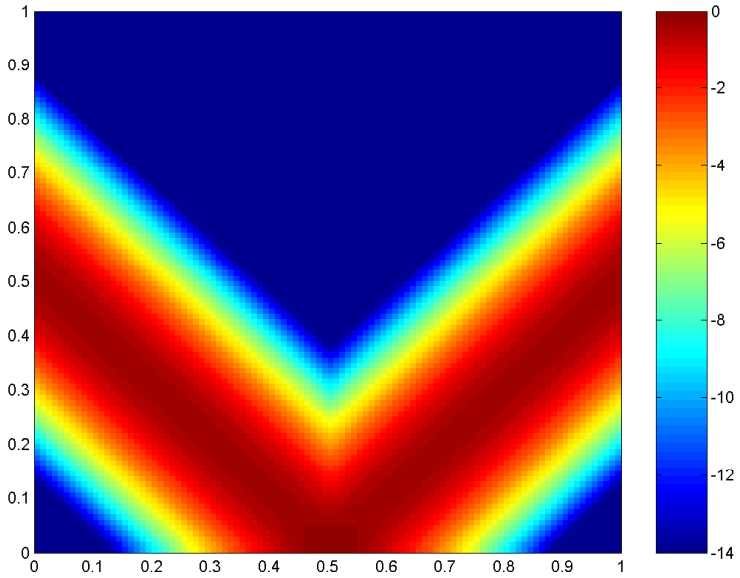

Figure 5.3: Logarithmic density plot of the solution, i.e. $\log_{10} u$, of (1.6) computed with the box scheme (2.10) and nonreflecting boundary conditions.

6. Conclusions

We have seen that nonphysical internal reflections arise from finite difference discretizations of the advection equation on nonuniform grids, whenever the numerical dispersion relation is non-monotone. Within the class of finite difference methods, only cell-centered differences can have monotone dispersion relations, and all such methods are necessarily implicit. Furthermore, we

have shown that symmetric Runge-Kutta methods, when applied to the spatial derivative of the advection equation, are reflection free.

For higher order wave equations, internal reflections can occur, even if the dispersion relation is monotone, due to coupling of characteristic modes for direct or staggered discretization of the higher order terms. Again, if a Runge-Kutta method is applied uniformly to a first order formulation of the wave equation (the approach of multisymplectic box schemes), the decoupling of characteristic modes is preserved by the discretization, and reflections do not occur.

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