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PROPAGATION AND REFLECTION IN DISCRETE-SPACE-DISCRETE-TIME STRUCTURES

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Abstract:

We describe the essential mathematics that are to be invoked to arrive at a coherent description of energy conservation, propagation and reflection in discrete-space-discrete-time structures. These are the structures which occur when hyperbolic equations are approximated numerically on a regular mesh in space-time.

The combined use of discrete Fourier Transforms and energy measures produces a set of new and particularly elegant results relating to spurious reflection at computational boundaries. These results are sketched in this paper.

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PROPAGATION AND REFLECTION IN DISCRETE-SPACE-DISCRETE-TIME STRUCTURES

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1. INTRODUCTION

The numerical approximation of hyperbolic equations generates structures which are discrete in time as well as in space. While space-periodic structures and wave propagation therein is a subject which is well understood and documented - see e.g. Brillouin (1946) - time-discretization is a subject that is essentially new, and its analysis has been carried out only in the recent past. The reason for this different state of affairs stems from the fact that while discrete-space periodic structures exist in the physical world (for instance in crystals, and in certain electrical networks), discrete-space-discrete-time structures are abstract entities, existing in symbolic form inside of certain numerical calculations which have become possible (or observable) only recently with the appearance of large electronic computers (in the 1950's and 60's). While many of the properties of discrete-time structures are similar to those of their continuous-time counterpart, there are also new aspects which are inherently introduced by the time-discretization.

We describe in this paper the essential mathematics that are to be invoked to arrive at a coherent description of a variety of phenomena which occur in those discrete structures. In particular, the combined use of discrete Fourier transforms and energy concepts produces a set of new and particularly elegant results relating to spurious reflection at computational boundaries and interfaces.

This paper is intended to be a general introduction. Details and proofs are to be found in the references cited.

2. DISCRETE-SPACE-DISCRETE-TIME STRUCTURES

Consider as a convenient model the simple hyperbolic equation

$$\frac{\partial U(x,t)}{\partial t} + c\,\frac{\partial U(x,t)}{\partial x} = 0 \qquad (1)$$

where c is a positive constant

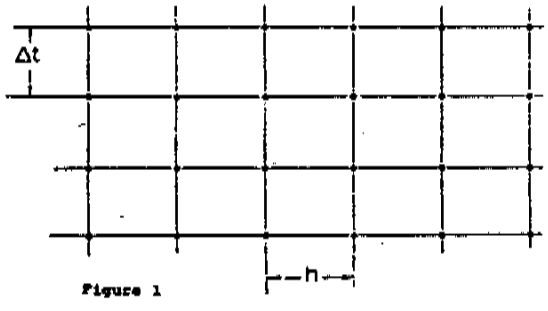

Figure 1

Consider also the regular mesh in (x, t) (figure 1):

$$\left.\begin{aligned} x_j &= jh\,;\ j = \cdots -1, 0, 1, 2 \cdots \\ t^n &= n\Delta t\,;\ n = \cdots -1, 0, 1, 2 \cdots \end{aligned}\right\} \qquad (2)$$

and the set of discrete values:

$$\{U_j^n\} = \{U(x_j, t^n)\} \qquad (3)$$

which is meant to approximate U. Simple numerical approximations of equation (1) may be obtained with finite differences by the two step process which consists in formulating at first a central-differences semi-discretization (CD)

$$\frac{dU_j}{dt} = -\frac{c}{2h}\left(U_{j+1} - U_{j-1}\right) \equiv A \cdot U_j \qquad (4)$$

and then in using a discrete time marching algorithm. This may be expressed by the general notation:

$$M(Z) \cdot U_n^j = A \cdot U_n^j \qquad (5)$$

where $M(\cdot)$, a discrete operator which approximates d/dt, contains the time-shift operator Z defined by:

$$U_j^{n+1} \equiv Z \cdot U_j^n \qquad (6)$$

We shall use as a model the simple trapezoidal (also called Crank Nicolson) scheme:

$$M(Z) = \frac{2}{\Delta t}\left(\frac{Z-1}{Z+1}\right) \qquad (7)$$

This will produce most of the essential results without unnecessary complications (see however section 10 for the description of other schemes).

3. WAVE PROPAGATION

The existence of wave propagation in the discrete structure described by (5) may be verified by inserting

$$U_j^n = e^{i(\omega n\Delta t + \xi j h)} \qquad (8)$$

into that equation. This results in

$$i\mu(\omega)\, U_j^n = -i\,\frac{c}{h}\sin(\xi h)\, U_j^n \qquad (9)$$

where $i\mu$ is the spectral function or symbol of the operator M defined as:

$$i\mu(\omega) \equiv \frac{M \cdot e^{i\omega n\Delta t}}{e^{i\omega n\Delta t}} \qquad (10)$$

and is obtained by simply replacing the operator

z by $e^{i\omega\Delta t}$ in the expression of M :

$$i\mu(\omega) = M(e^{i\omega\Delta t}) \qquad (11)$$

Time discretization methods for which $i\mu$ has no real part:

$$Re(i\mu(\omega)) = 0 \qquad (12)$$

may have solutions of the form (8) where ω and ξ both real, are related by the dispersion relation derived from (9):

$$\mu(\omega) = -\frac{c}{h}\sin(\xi h) \qquad (13)$$

Equation (8) then describes sinusoidal solutions of constant amplitude in both space and time. It may be verified that (12) holds for (7) with

$$\mu(\omega) = \frac{2}{\Delta t}\tan\left(\frac{\omega\Delta t}{2}\right) \qquad (14)$$

Moreover, solving the dispersion relation (13) for ω results in

$$\text{real valued } \omega \text{ for all real valued } \xi \qquad (15)$$

The algorithm (5)-(7) thus admits constant amplitude sinusoidal waves for all $|\xi|$ in $[0,\pi/h]$. It is therefore called energy conservative for reasons that come from the context of the mathematics of section 4.
Since M is an approximation of d/dt, it is also the case that

$$\lim_{\Delta t \to 0} \mu(\omega) = \omega \qquad (16)$$

This property is the Fourier-space form of the consistency condition of M, as defined in classical numerical analysis - see e.g. Richtmyer and Morton (1967) for such a classical definition.

4. FOURIER TRANSFORMS

To obtain precise results, in particular those expressing energy propagation, one must abandon the use of "sinusoidal trial solutions" and replace it with Fourier integrals. The analysis is restricted to functions which are in a Hilbert space, i.e. for which the ℓ_2 norm

$$\|U_j^n\|_2 = \left(h\sum_{j=-\infty}^{\infty}|U_j^n|^2\right)^{1/2} \qquad (17)$$

is finite. It is convenient to refer to the square of this quantity as the "energy" of U :

$$\mathcal{E}^n = \|U_j^n\|_2^2 = h\sum_j |U_j^n|^2 \qquad (18)$$

One may define Fourier transforms in x and t, and repeat an analysis of propagation characteristics comparable to that of section 3. The results are summarized in Tables 1. and 2.

To each $|\omega|$ in a passing band bounded from above by some maximum value ω_c, there exist two types of solutions:

- a solution with wave number $|\xi_1|$ in $[0,\pi/2h)$ or wavelength λ in $(4h,\infty)$ and a positive group velocity (called solution of p type)

- and a solution with wave number $|\xi_2|$ in $(\pi/2h,\pi/h]$ or wavelength λ in $[2h,4h)$ and negative group velocity (called solution of q type).

Note that discrete (instead of continuous) Fourier transforms are being used. While this tool is non-standard in numerical analysis (is is mostly used by engineers), its use here results in exact expressions of energy, whereas continuous transforms give only assymptotic approximations - see [23] for a detailed analysis.

Analysis of propagation with x-Fourier transforms

x-Fourier Transform :

$$\overline{U}^n(\xi) = h\sum_j U_j^n e^{-i\xi jh} \quad ; |\xi| \le \pi/h$$

Amplification factor :

$$z(\xi) = \overline{U}^{n+1}(\xi)/\overline{U}^n(\xi)$$

is a solution of the characteristic equation :

$$M(z(\xi)) = -i\frac{c}{h}\sin(\xi h)$$

(the solution satisfies $|z| = 1$ for energy conservative schemes, by the converse of (15))

Dispersion relation :

$$\omega\Delta t = \angle z(\xi)$$

Group velocity :

$$G(\xi) = -\frac{1}{\Delta t}\frac{d}{d\xi}\angle z(\xi)$$

Energy: (Parseval's relation)

$$\mathcal{E}^n = \|U_j^n\|_2^2 = h\sum_j |U_j^n|^2 = \int_0^{\pi/h}|\overline{U}^n(\xi)|^2\frac{d\xi}{\pi}$$

Table 1

Analysis of propagation with t-Fourier transforms

t-Fourier Transform :

$$\overline{U}_j(\omega) = \Delta t\sum_n U_j^n e^{-i\omega n\Delta t} \quad ; |\omega| \le \pi/\Delta t$$

x-Amplification factor (also called cell-transfer function)

$$\hat{E}(\omega) = \overline{U}_{j+1}(\omega)/\overline{U}_j(\omega)$$

is a solution of the characteristic equation:

$$\hat{E}^2 + 2i\mu(\omega)\frac{h}{c}\hat{E} - 1 = 0$$

Dispersion relation :

$$\xi h = \angle\hat{E}(\omega)$$

Group velocity :

$$G(\omega) = -\frac{1}{h}\left(\frac{d\angle\hat{E}}{d\omega}\right)^{-1} = c\sqrt{1-\left(\mu(\omega)\frac{h}{c}\right)^2}\frac{d\omega}{d\mu}$$

Energy flow across x_j :

$$\mathcal{E}_j = \int_0^{\pi/\Delta t}|\overline{v}_j(\omega)|^2 G(\omega)\frac{d\omega}{\pi}$$

Table 2

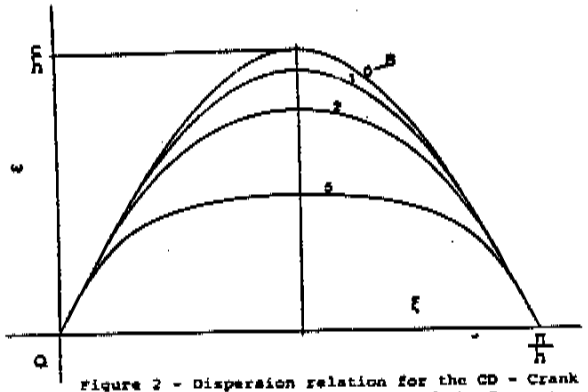

Figure 2 - Dispersion relation for the CD - Crank Nicolson Scheme-different values of the Courant number $R = c\Delta t/h$

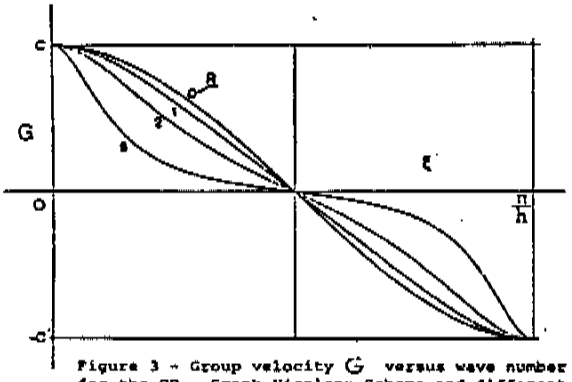

Figure 3 - Group velocity G versus wave number ξ for the CD - Crank Nicolson Scheme and different values of the Courant number R

Finite Domains

We have so far described wave propagation in discrete-space-discrete-time structures defined on $(-\infty, \infty)$. In most problems of interest, waves and energy are defined on semi-infinite or finite instead of infinite spaces: it may be verified that most of the tools used so far do apply to those cases with little or no modification. Indeed it suffices to assume that all variables on non-infinite domains do indeed exist on $(-\infty, \infty)$, but that their numerical value is equal to zero outside of their own domain of definition. For instance, for a function defined on the half space

$$D = [0, \infty) \quad (\text{or } j \in [0, \infty)) \tag{19}$$

the following definitions of its Fourier transform, its energy and their relationship through Parseval's relation

$$\overline{u}(\xi) = h \sum_{j \geq 0} u_j e^{-i\xi jh} \tag{20}$$

$$\epsilon = h \sum_{j \geq 0} |u_j|^2 = \int_0^{\pi/h} |\overline{u}(\xi)|^2 \frac{d\xi}{\pi} \tag{21}$$

are observed to apply strictly once the above is invoked. And similar extensions hold with t-Fourier transforms, for functions which are defined for $t \geq 0$ only.

5. BOUNDARIES

When a discrete structure of the form defined by (5) is implemented on a finite domain, say

$$D = [-\ell, 0] \tag{22}$$

then it may be noted that (5) cannot be applied in the boundary points $-\ell$ and 0. What this means is that in addition to initial data in D, boundary data must be given in $-\ell$ and 0 to specify the solution.

We note that in contrast, specifying a solution of (1) requires only one boundary condition (in $-\ell$). That two boundary conditions are needed by (5) reflects the fact that this structure is of second order. Indeed, it may be shown that when h and Δt are made to tend to zero in an appropriate way, then, in the limit, solutions of (5) tend to solutions of the second order wave equation [21,23]:

$$\frac{\partial^2 U}{\partial t^2} - c^2 \frac{\partial^2 U}{\partial x^2} = 0 \tag{23}$$

The class of functions which are solutions of this equation does contain the solutions of (1). But it contains also solutions of

$$\frac{\partial U}{\partial t} - c \frac{\partial U}{\partial x} = 0 \tag{24}$$

The discrete analog of these solutions are precisely those which are described as being of q type in the Fourier analysis. And the additional boundary condition needed by the discrete structure at the "downwind" boundary $x = 0$ is that which correspond to those solutions.

Downwind Boundaries

When (5) is used as a numerical algorithm to approximate solutions of (1), then the implicit assumption is that no solution of (24) should be present. This is equivalent to saying that (1) applies at the boundary. It is interesting, but not unexpected, to note that our original equation is precisely what is called the Sommerfeld Radiation Condition for the wave equation (23) (see e.g. Courant and Hilbert (1962) - Vol. II, Pg. 315).

A discrete approximation of equation (1) which is implementable in $x = 0$ is the usual 2 point "upwind" equation:

$$M \cdot u_0^n = -\frac{c}{h}\left(u_0^n - u_{-1}^n\right) \tag{25}$$

where M is the same as in (5). Because of this different treatment at the boundary, reflection occurs: The question is conveniently analysed in Fourier space.

It must be noted that the appropriate tool for this kind of analysis is that of t-Fourier transforms; x-Fourier transforms do not work. The reason for this stems from the fact that the frequency (ω) (the dual variable of t-Fourier transforms) is an invariant: it remains constant when a wave encounters a discontinuity, while the wave number does not. (One finds interesting comments in Brillouin (1946) which are parallel to this: Brillouin credits Kelvin (1881) with the introduction of the frequency (instead of wave number) as an independent variable in the analysis of wave propagation in lattice structures, thereby succeeding in obtaining many new results, inparticular

those concerning the multiplicity of waves and their respective interactions.) Reflection occurs when a rightgoing solution (of p type), which originates from D arrives at the boundary x=0. During its passage through that point, it generates a leftgoing solution (of q type) which returns toward D.

Denoting by $\overline{p_0}(\omega)$ and $\overline{q_0}(\omega)$ the respective t-Fourier transforms at the boundary, we have:

$$\overline{U_0}(\omega) = \overline{p_0}(\omega) + \overline{q_0}(\omega) \qquad (26)$$

Expressing the Fourier transform of (25), and solving for q/p then results in

$$\rho(\omega) \equiv \frac{\overline{q_0}(\omega)}{\overline{p_0}(\omega)} = -\frac{1+i\mu h/c - \widehat{E_1}^{-1}}{1+i\mu h/c - \widehat{E_2}^{-1}} \qquad (27)$$

where ρ is called the amplitude reflection ratio.

The wave number of an incident and reflected solution are those which correspond to the same value of ω through the dispersion relation (13),

$$|\xi_2| = \frac{\pi}{h} - |\xi_1| \qquad (28)$$

Of interest is the case of a "smooth" incident wave which may be considered as a packet of wave number ξ_1 near 0. The reflected solution is then also a wave packet, of wave number $|\xi_2|$ near π/h, i.e. of wave length near $2h$.

Those reflected waves have a typical saw-toothed appearance, as illustrated by the numerical experiment whose results are shown in figure 4.

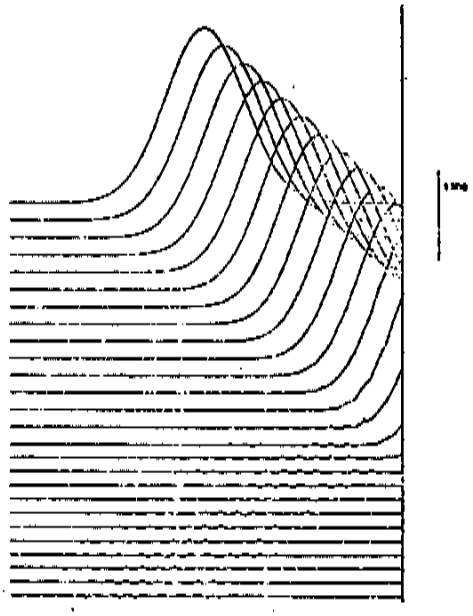

Figure 4 - Reflection at a downwind boundary by equation (25). The sawtoothed nature of the reflected wave packet is clearly visible - (from Vichnevetsky and Pariser - ref. [22]).

6. ENERGY REFLECTION

One may quantify the performance of a boundary equation such as (25) by the energy that it reflects in response to an arbitrary rightgoing solution which originates from D. To illustrate this, consider the domain $(-\infty, 0]$ for the CD - Crank Nicolson scheme and (25) at the right boundary, with an imposed initial condition assumed to contain only a rightgoing component.

As $t \to \infty$, this function has passed entirely across the boundary, and the energy remaining in D is that which has been reflected. We may express this energy as:

$$\mathcal{E}_R = \lim_{n\to\infty} \mathcal{E}^n = \int_0^{\omega_c} |\overline{p_0}(\omega)\,\rho(\omega)|^2 G(\omega)\frac{d\omega}{\pi} \qquad (29)$$

Where $\overline{p_0}(\omega)$ is related to the initial conditions by the relation

$$|\overline{p_0}(\omega)| = |\overline{p^0}(\xi)/G(\xi)| \qquad (30)$$

(see [17,18] for details).

7. INVARIANCE PROPERTIES

Interesting, and somewhat unexpected properties concern the independence of energy reflection at boundaries from the specifics of how time marching is being implemented. What the following results will show is that the energy reflectod at boundaries is in many respects a function only of how $\partial/\partial x$ is approximated. I.e., this energy is independent of the form of the time-marching operator M (as long as essential conservation and stability properties are preserved).

The following is intended to be only a sketchy description of those results. Precise derivations may be found elsewhere [20].

> Theorem 1: For the structure of Sec 6, the energy reflected at the boundary as $t \to \infty$ is independent of Δt, and is strictly equal to the energy reflected in the semi-discrete system obtained when M is replaced by d/dt.

The proof consists in verifying that when $\mathcal{E}_R$ is expressed by an integral in x-Fourier space (instead of (29)), then this expression becomes independent of Δt, and is identical to the expression of the energy reflected in the semi-discrete case, i.e. when $\mu(\omega) \equiv \omega$.

Given in figure 5 are the results of a numerical experiment which illustrates this invariance property: the reflection of a Gaussian initial $U(x,0)$ in D by the boundary equation (25) has been repeated with values of R corresponding to a Courant number R=0.1, 1., 3. and 5.

In each case, plotted is the energy $\mathcal{E}^n$ versus time (n). While figure 5 shows that the numerical solution (and the energy) is evidently affected by changes in R, it is nevertheless the case that $\mathcal{E}_R$ (which is the asymptotic value of $\mathcal{E}^n$ when $n \to \infty$) is the same in all cases. This constant value was also verified to agree (to within arithmetical accuracy, i.e. 10 significant digits in double precision calculations on a 36 bit computer) with the integral (29) evaluated by numerical quadrature.

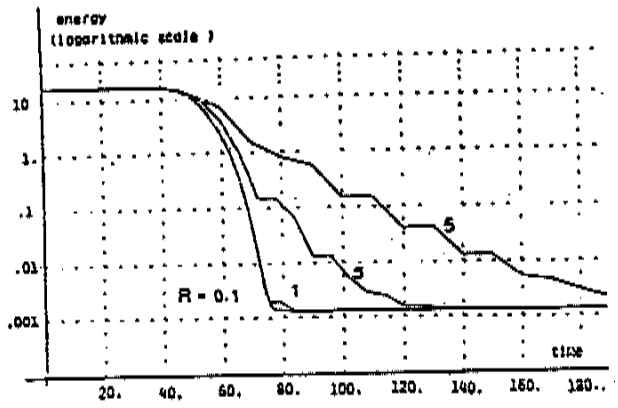

Figure 5 - Energy versus time for the calculation illustrated in Figure 4, and different values of the Courant number R. The asymptotic value $\mathcal{E}_A$ of the energy is strictly independent of R.

While Theorem 1 has been stated in the specific case of the CD - Crank Nicolson scheme, there are obvious extensions: The invariance will continue to apply when other energy conservative, stable algorithms are used (simple examples are easily constructed).

8. CONVERGENCE

Even more generality of the preceding result is obtained when Theorem 1 is recast in the language of convergence analysis:

Given an initial function $U(x,0)$ in D, sampled at the mesh points,

$$U_j^0 = U(jh,0) \; ; \quad j < 0 \qquad (31)$$

for the scheme (5), (7), (25),

- and the limiting process $h \to 0$, $\Delta t \to 0$ (in any manner), then

> Theorem 2: The rate of convergence to zero of the reflected energy $\mathcal{E}_R$ is the same as that of the semi-discrete scheme ($M = d/dt$) when $h \to 0$.

While this theorem is an obvious rephrasing of Theorem 1, it leads to more general results: We note that when $\Delta t \to 0$, then $U \to u$ not only for the Crank-Nicolson method, but also for any other consistent (not necessarily energy conservative) time-integration algorithm applied to (4); we may thus state (with minor modifications of definitions, e.g. imposing that $U(x,0)$ be, to within a remainder of negligible energy, of finite support in D and letting $\mathcal{E}_A = \mathcal{E}^J$ where J is sufficiently large, but finite):

> Theorem 3: Theorem 2 applies not only to the CD - Crank Nicolson scheme, but also to other schemes obtained when any consistent, not necessarily energy conservative time-marching algorithm M is used in (5)-(25).

The only caveat is that stability must be preserved. An example is given in section 10 below.

9. HIGH ORDER NON REFLECTING BOUNDARIES

One may want to reduce reflection at a downwind boundary by the use of higher order equations. I.e., instead of (25), the equation

$$\mathcal{B} \equiv M \cdot U_0^n - a_0 U_0^n - a_1 U_{-1}^n - a_2 U_{-2}^n \cdots = 0 \qquad (32)$$

limited to a specified number of terms is of an order greater than (25) when more than 2 terms are used.

A point of semantics: the term "order" used here refers to the standard method used to generate the free coefficients in (32); since that equation is meant, in some sense, to approximate the Sommerfeld radiation condition (1), one may use Taylor series to express the terms of (32) round (x_0, t^n), and use the free coefficients to match as many terms as possible with (1). The "order" is then that of this approximation in the classical numerical analysis sense.

There is, however, a different approach to the synthesis of (32) which is more correct. It consists in recognizing that lack of reflection in the discrete structure corresponds to the ideal $\rho = 0$ (which is a discrete form of Sommerfeld's condition consistent with the actual discrete equations).

Expressing ρ for (32) and then finding the free coefficients which maximize the number of zero terms in its Taylor Series expansion near $\omega = 0$ produces the same results as the classical method when 2 or 3 terms are used, but gives different results beyond. As expected, the performance of those "discrete Sommerfeld" high order schemes, measured by the smallness of energy reflection, is superior to the standard schemes. ([22]). (See also Halpern (1982) for a similar synthesis of boundary equations for numerical approximations of the wave equation.) In the implementation of this procedure, we are led to making use of Theorem 3 (suitably generalized, with equation (25) replaced by (32)). As a consequence, one may develop high-order non-reflecting formulae for the semi-discrete system (4)

$$\mathcal{B}_s \equiv \frac{du_0}{dt} - a_0 u_0 - a_1 u_{-1} - a_2 u_{-2} \cdots = 0 \qquad (33)$$

and be assured that their non-reflection properties, measured in the energy norm, remain unchanged when time integration is implemented with Crank-Nicolson, or any other consistent time marching method (as long as stability is preserved).
See Vichnevetsky and Pariser (1984) - in which details and numerical experiments may be found.

10. ADDITIONAL COMMENTS

Since only one scheme has been considered in our analysis, (the CD - Crank Nicolson), it may be useful to ask which of the specific results may generalize to other cases, and what new properties may result from the analysis of such other cases.

Some answers are obtained by considering two characteristic examples.

First the leapfrog scheme, which is of the form (5), with

$$M \cdot = \frac{1}{2\Delta t}\left(Z - Z^{-1}\right). \qquad (34)$$

(cf. Richardson - 1910 for a first description of this algorithm given in the context of the numerical approximation of parabolic equations). This scheme illustrates modes of instability not present in the Crank Nicolson case. The Cauchy instability which occurs when $R > 1$ is well known (cf. Courant, Friedrichs and Lewy-1928). Another mode of instability occurs at the boundaries: see ref. [11] for a classical analysis, and Trefethen (1983) for an analysis using the concepts of reflection and group velocity.

A second example is the predictor-corrector:

$$\left.\begin{aligned} U_j^p &= U_j^n + \Delta t\, A \cdot U_j^n \\ U_j^{n+1} &= U_j^n + \Delta t\, A \cdot U_j^p \end{aligned}\right\} \qquad (35)$$

which may also be expressed as (instead of (5)):

$$(Z - 1)\cdot U_j^n = \left(\Delta t\, A + (\Delta t A)^2\right)\cdot U_j^n$$

(This is the first order Adams Bashforth method applied to the semi discrete equations (4)). The scheme is dissipative and stable when $R \leq 1$ (ref. [23]). It may serve as an example to illustrate Theorem 3. Indeed, while not energy conservative, it is nevertheless the case that the behavior of this scheme becomes identical to that of the Crank Nicolson in the limit of the converging sequence for which the Theorem holds true.

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