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## THEORETICAL OPTIMIZATION OF FINITE DIFFERENCE SCHEMES

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ABSTRACT. The aim of this work is to develop general optimization methods for finite difference schemes used to approximate linear differential equations. The specific case of the transport equation is exposed. In particular, the minimization of the numerical error is taken into account. The theoretical study of a related linear algebraic problem gives general results which can lead to the determination of the optimal scheme.

**1. Introduction: Scheme classes.** Finite difference schemes used to approximate linear differential equations induce numerical errors, that are generally difficult to predict. The usual process consists in testing various schemes for more and more refined time and space steps.

We here propose a completely different approach, which consists in determining the minimum norm error of a given finite difference scheme. This process has the advantage of avoiding scheme convergence tests. Moreover, it can explain error jumps that often occur in such approximations.

Consider the transport equation:

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \tag{1}$$

with the initial condition  $u(x, t = 0) = u_0(x)$ .

A finite difference scheme for this equation can be written under the form:

$$\alpha u_i^{n+1} + \beta u_i^n + \gamma u_i^{n-1} + \delta u_{i+1}^n + \varepsilon u_{i-1}^n + \zeta u_{i+1}^{n+1} + \eta u_{i-1}^{n-1} + \theta u_{i-1}^{n+1} + \vartheta u_{i+1}^{n-1} = 0 \tag{2}$$

where:

$$u_l^m = u(lh, m\tau) \tag{3}$$

$l \in \{i-1, i, i+1\}$ ,  $m \in \{n-1, n, n+1\}$ ,  $j = 0, \dots, n_x$ ,  $n = 0, \dots, n_t$ ,  $h$ ,  $\tau$  denoting respectively the mesh size and time step.

The Courant-Friedrichs-Lewy number ( $cfl$ ) is defined as  $\sigma = c\tau/h$ .

A numerical scheme is specified by selecting appropriate values of the coefficients  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$ ,  $\varepsilon$ ,  $\zeta$ ,  $\eta$ ,  $\theta$  and  $\vartheta$  in equation (2). Values corresponding to numerical schemes retained for the present works are given in Table 1.

TABLE 1. Numerical scheme coefficient.

| Name           | $\alpha$                         | $\beta$                                 | $\gamma$           | $\delta$                          | $\epsilon$                        | $\zeta$ | $\eta$           | $\theta$         | $\vartheta$ |
|----------------|----------------------------------|---|--------------------|-----------------------------------|-----------------------------------|---------|------------------|------------------|-------------|
| Leapfrog       | $\frac{1}{2\tau}$                | 0                                       | $\frac{-1}{2\tau}$ | $\frac{c}{2h}$                    | $\frac{-c}{2h}$                   | 0       | 0                | 0                | 0           |
| Lax            | $\frac{1}{\tau}$                 | 0                                       | 0                  | $\frac{-1}{2\tau} + \frac{c}{2h}$ | $\frac{-1}{2\tau} - \frac{c}{2h}$ | 0       | 0                | 0                | 0           |
| Lax-Wendroff   | $\frac{1}{\tau}$                 | $\frac{-1}{\tau} + \frac{c^2\tau}{h^2}$ | 0                  | $\frac{(1-\sigma)c}{2h}$          | $\frac{-(1+\sigma)c}{2h}$         | 0       | 0                | 0                | 0           |
| Crank-Nicolson | $\frac{1}{\tau} + \frac{c}{h^2}$ | $\frac{-1}{\tau} + \frac{c}{h^2}$       | 0                  | $\frac{2h}{h^2}$                  | $\frac{-c}{h^2}$                  | 0       | $\frac{-c}{h^2}$ | $\frac{-c}{h^2}$ | 0           |

The number of time steps will be denoted  $n_t$ , the number of space steps,  $n_x$ . In general,  $n_t \gg n_x$ .

The paper is organized as follows. The equivalent matrix equation is exposed in section 2. Scheme optimization is presented in section 3.

## 2. The Sylvester equation.

**2.1. Matricial form of the finite differences problem.** Let us introduce the rectangular matrix defined by:

$$U = [u_i^n]_{1 \leq i \leq n_x - 1, 1 \leq n \leq n_t} \quad (4)$$

The problem (2) can be written under the following matricial form:

$$M_1 U + U M_2 + \mathcal{L}(U) = M_0 \quad (5)$$

where  $M_1$ ,  $M_2$  and  $M_0$  are square matrices respectively  $n_x - 1$  by  $n_x - 1$ ,  $n_t$  by  $n_t$ , given by:

$$M_1 = \begin{pmatrix} \beta & \delta & 0 & \dots & 0 \\ \epsilon & \beta & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \beta & \delta \\ 0 & \dots & 0 & \epsilon & \beta \end{pmatrix} \quad M_2 = \begin{pmatrix} 0 & \gamma & 0 & \dots & 0 \\ \alpha & 0 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma \\ 0 & \dots & 0 & \alpha & 0 \end{pmatrix} \quad (6)$$

$$M_0 = \begin{pmatrix} -\gamma u_1^0 - \epsilon u_0^1 - \eta u_0^0 - \theta u_0^2 - \vartheta u_2^0 & -\epsilon u_0^2 - \eta u_0^1 - \theta u_0^3 & \dots & \dots & -\epsilon u_0^{n_t} - \eta u_0^{n_t-1} \\ -\gamma u_2^0 - \eta u_1^1 - \vartheta u_3^0 & 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -\gamma u_{n_x-2}^0 - \eta u_{n_x-2}^1 - \vartheta u_{n_x-1}^0 & 0 & \dots & \dots & 0 \\ -\gamma u_{n_x-1}^0 - \delta u_{n_x}^1 - \eta u_{n_x-2}^0 - \zeta u_{n_x}^2 - \vartheta u_{n_x}^0 & -\delta u_{n_x}^2 - \zeta u_{n_x}^3 - \vartheta u_{n_x}^1 & \dots & \dots & -\delta u_{n_x}^{n_t} - \vartheta u_{n_x}^{n_t-1} \end{pmatrix} \quad (7)$$

and where  $\mathcal{L}$  is a linear matricial operator which can be written as:

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4 \quad (8)$$

where  $\mathcal{L}_1$ ,  $\mathcal{L}_2$ ,  $\mathcal{L}_3$  and  $\mathcal{L}_4$  are given by:

$$\mathcal{L}_1(U) = \zeta \begin{pmatrix} u_2^2 & u_2^3 & \dots & u_2^{n_t} & 0 \\ u_3^2 & u_3^3 & \dots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u_{n_x-1}^2 & u_{n_x-1}^3 & \dots & u_{n_x-1}^{n_t} & 0 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix} \quad \mathcal{L}_2(U) = \eta \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ 0 & u_1^1 & u_1^2 & \dots & u_1^{n_t-1} \\ 0 & u_1^0 & u_1^1 & \dots & u_2^{n_t-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & u_{n_x-2}^1 & u_{n_x-2}^2 & \dots & u_{n_x-2}^{n_t-1} \end{pmatrix} \quad (9)$$

$$\mathcal{L}_3(U) = \theta \begin{pmatrix} 0 & \dots & \dots & \dots & 0 \\ u_1^2 & u_1^3 & \dots & u_1^{n_t} & 0 \\ u_2^2 & u_2^3 & \dots & u_2^{n_t} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{n_x-2}^2 & u_{n_x-2}^3 & \dots & u_{n_x-2}^{n_t} & 0 \end{pmatrix} \quad \mathcal{L}_4(U) = \vartheta \begin{pmatrix} 0 & u_2^1 & u_2^2 & \dots & u_2^{n_t-1} \\ 0 & u_3^1 & u_3^2 & \dots & u_3^{n_t-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & u_{n_x-1}^1 & \dots & \dots & u_{n_x-1}^{n_t-1} \\ 0 & 0 & \dots & \dots & 0 \end{pmatrix} \quad (10)$$

The second member matrix  $M_0$  bears the initial conditions, given for the specific value  $n = 0$ , which correspond to the initialization process when computing loops, and the boundary conditions, given for the specific values  $i = 0$ ,  $i = n_x$ .

Denote by  $u_{exact}$  the exact solution of (1).  
The  $U_{exact}$  corresponding matrix will be:

$$U_{exact} = [U_{exact_i}^n]_{0 \leq i \leq n_x-1, 0 \leq n \leq n_t} \quad (11)$$

where:

$$U_{exact_i}^n = U_{exact}(x_i, t_n) \quad (12)$$

with  $x_i = i h$ ,  $t_n = n \tau$ .

$U$  is then solution of:

$$M_1 U + U M_2 + \mathcal{L}(U) = M_0 \quad (13)$$

We will call *error matrix* the matrix defined by:

$$E = U - U_{exact} \quad (14)$$

Let us consider the matrix  $F$  defined by:

$$F = M_1 U_{exact} + U_{exact} M_2 + \mathcal{L}(U_{exact}) - M_0 \quad (15)$$

The *error matrix*  $E$  satisfies then:

$$M_1 E + E M_2 + \mathcal{L}(E) = F \quad (16)$$

## 2.2. The matrix equation.

2.2.1. *Theoretical formulation.* Minimizing the error due to the approximation induced by the numerical scheme is equivalent to minimizing the norm of the matrices  $E$  satisfying (16).

Since the linear matricial operator  $\mathcal{L}$  appears only in the Crank-Nicholson scheme, we will restrain our study to the case  $\mathcal{L} = 0$ . The generalization to the case  $\mathcal{L} \neq 0$  can be easily deduced.

The problem is then the determination of the minimum norm solution of:

$$M_1 E + E M_2 = F \quad (17)$$

which is a specific form of the Sylvester equation:

$$AX + XB = C \quad (18)$$

where  $A$  and  $B$  are respectively  $m$  by  $m$  and  $n$  by  $n$  matrices,  $C$  and  $X$ ,  $m$  by  $n$  matrices.

The solving of the Sylvester equation is generally based on Schur decomposition: for a given square  $n$  by  $n$  matrix  $A$ ,  $n$  being an even number of the form  $n = 2p$ , there exists a unitary matrix  $U$  and a upper triangular block matrix  $T$  such that:

$$A = U^* T U \quad (19)$$

where  $U^*$  denotes the (complex) conjugate matrix of the transposed matrix  $^T U$ . The diagonal blocks of the matrix  $T$  correspond to the complex eigenvalues  $\lambda_i$  of  $A$ :

$$T = \begin{pmatrix} T_1 & 0 & \dots & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & T_i & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & T_p \end{pmatrix} \quad (20)$$

where the block matrices  $T_i$ ,  $i = 1, \dots, p$  are given by:

$$\begin{pmatrix} \mathcal{R}e[\lambda_i] & \mathcal{I}m[\lambda_i] \\ -\mathcal{I}m[\lambda_i] & \mathcal{R}e[\lambda_i] \end{pmatrix} \quad (21)$$

$\mathcal{R}e$  being the real part of a complex number, and  $\mathcal{I}m$  the imaginary one.

Due to this decomposition, the Sylvester equation require, to be solved, that the

dimensions of the matrices be even numbers. We will therefore, in the following, restrain our study to  $n_x$  and  $n_t$  being even numbers. So far, it is interesting to note that the Schur decomposition being more stable for higher order matrices, it perfectly fits finite differences problems.

Complete parametric solutions of the generalized Sylvester equation (??) is given in [2], [3].

As for the determination of the solution Sylvester equation, it is a major topic in control theory, and has been the subject of numerous works (see [1], [6], [8], [9], [10], [11], [12]).

In [1], the method is based on the reduction of the he observable pair  $(A, C)$  to

an observer-Hessenberg pair  $(H, D)$ ,  $H$  being a block upper Hessenberg matrix. The reduction to the observer-Hessenberg form  $(H, D)$  is achieved by means of the staircase algorithm (see [4], ...).

In [9], in the specific case of  $B$  being a companion form matrix, the authors propose a very neat general complete parametric solution, which is expressed in terms of the controllability of the matrix pair  $(A, B)$ , a symmetric matrix operator, and a parametric matrix in the Hankel form.

We recall that a companion form, or Frobenius matrix is one of the following kind:

$$B = \begin{pmatrix} 0 & \dots & \dots & \dots & 0 & -b_0 \\ 1 & 0 & \dots & \dots & 0 & -b_1 \\ 0 & 1 & 0 & \dots & \vdots & \vdots \\ \vdots & 0 & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & -b_{p-1} \end{pmatrix} \quad (22)$$

These results can be generalized through matrix block decomposition to a block companion form matrix, which happens to be the case of our matrix  $M_2$  in the specific case of  $n_x$  and  $n_t$  being even numbers:

$$M_2 = \begin{pmatrix} M_2^{B^1} & 0 & \dots & \dots & 0 \\ 0 & M_2^{B^2} & 0 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & M_2^{B^k} \end{pmatrix} \quad (23)$$

the  $M_2^{B^p}$ ,  $1 \leq p \leq k$  being companion form matrices.

Another method is presented in [14], where the determination of the minimum-norm solution of a Sylvester equation is specifically developed.

The accuracy and computational stability of the solutions is examined in [5].

*2.2.2. Existence condition of the solution.* Equation (18) has a unique solution if and only if  $A$  and  $B$  have no common eigenvalues.

In our case, since  $M_2$  is a upper triangular matrix whose diagonal coefficients are all equal to  $\alpha$ , its eigenvalues are also all equal to  $\alpha$ . As for the matrix  $M_1$ , one can easily check that  $\alpha$  does not belong to its spectra. Hence, (16) has a unique solution, which accounts for the consistency of the given problem.

**3. Scheme optimization.** Advect a sinusoidal signal

$$u = \text{Cos} \left[ \frac{2\pi}{\lambda} (x - ct) \right] \quad (24)$$

through the Lax scheme, where:

$$\lambda = n_\lambda dx \quad (25)$$

$n_\lambda$  denotes the number of cells per wavelength.

Let  $n_\lambda$  remain unknown.

Equation (17) can thus be normalized as:

$$\overline{M}_1 E + E \overline{M}_2 = \overline{F} \quad (26)$$

where

$$\begin{cases} \overline{M}_1 &= \frac{h c fl}{c} M_1 \\ \overline{M}_2 &= \frac{h c fl}{c} M_2 \\ \overline{F} &= \frac{h c fl}{c} F \end{cases} \quad (27)$$

We deliberately choose a small value for the number of steps:  $n_t = n_x = 20$ , starting from the point that if the error is minimized for a small value of this number, it will be the same as this number increases.

Figure displays the  $L_2$  norm of the isovalues of the error as a function of  $n_\lambda$  (maximums are in white, minimums in black; larger values are shown lighter).

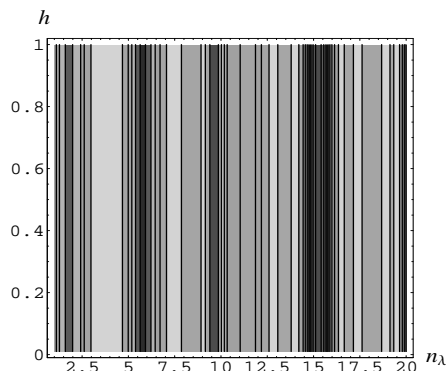


FIGURE 1. Isovalues of the  $L_2$  norm of the error as a function of the number of cells per wavelength  $n_\lambda$

The square value of the  $L_2$  norm of the error, for two significative values of the number of cells per wavelength  $n_p$ , is displayed in Figure 2:

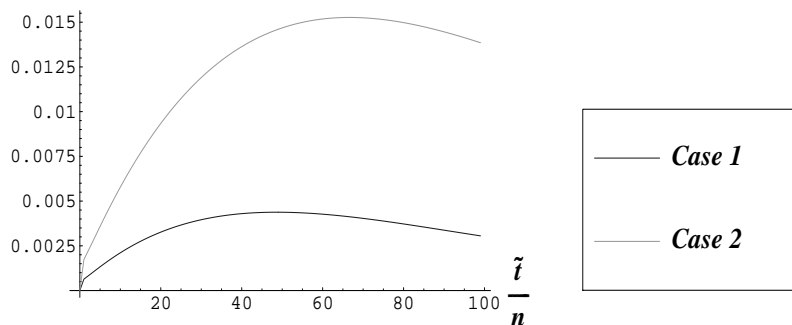


FIGURE 2. square value of the  $L_2$  norm of the error as a function of the number of cells per wavelength  $n_\lambda$ . Case 1:  $\lambda = 9$ . Case 2:  $\lambda = 9.8$ .

The above results ensure the faster convergence of the error.

**4. Conclusion.** Thanks to the above results, we presently propose to optimize finite difference problems through minimization of the symbolic expression of the error as a function of the scheme parameters.

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