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FINITE DIFFERENCE SCHEMES AS A MATRIX EQUATION

CLAIRE DAVID AND PIERRE SAGAUT*

Abstract.

Finite difference schemes are here solved by means of a linear matrix equation. The theoretical study of the related algebraic system is exposed.

Key words. Finite difference schemes, Sylvester equation

AMS subject classifications. 15A15, 15A09, 15A23

1. Introduction: Scheme classes. Finite difference schemes used to approximate linear differential equations are usually solved by means of a recursive calculus, expensive in time and not of practical handling.

We here propose a completely different approach, which consists in solving an equivalent matrix equation.

Consider the transport equation:

(1.1)
$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 , x \in [0, L], t \in [0, T]$$

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

Proposition 1.1.

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

$$\alpha\,u_{i}{}^{n+1} + \beta\,u_{i}{}^{n} + \gamma\,u_{i}{}^{n-1} + \delta\,u_{i+1}{}^{n} + \varepsilon\,u_{i-1}{}^{n} + \zeta\,u_{i+1}{}^{n+1} + \eta\,u_{i-1}{}^{n-1} + \theta\,u_{i-1}{}^{n+1} + \vartheta\,u_{i+1}{}^{n-1} = 0 \eqno(1.2)$$
 where:

$$(1.3) u_l^m = u(l\,dx, m\,dt)$$

 $l \in \{i-1, i, i+1\}, m \in \{n-1, n, n+1\}, j=0, ..., n_x, n=0, ..., n_t, dx, dt$ denoting respectively the mesh size and time step $(L = n_x dx, T = n_t dt)$. The Courant-Friedrichs-Lewy number (cfl) is defined as $\sigma = cdt/dx$.

A numerical scheme is specified by selecting appropriate values of the coefficients α , β , γ , δ , ε , ζ , η , θ and ϑ in equation (1.2). Values corresponding to numerical schemes retained for the present works are given in Table 1.1.

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

The paper is organized as follows. The equivalent matrix equation is exposed in section 2. Specific properties of the involved matrices are exposed in section 2.3.

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Table 1.1
Numerical scheme coefficient.

Name	α	β	γ	δ	ϵ	ζ	η	θ	ϑ
Leapfrog	$\frac{1}{2\tau}$	0	$\frac{-1}{2\tau}$	$\frac{c}{2h}$	$\frac{-c}{2h}$	0	0	0	0
Lax	$\frac{\gamma}{\tau}$	0	0	$\frac{-1}{2\tau} + \frac{c}{2h}$	$\frac{-1}{2\tau} - \frac{c}{2h}$	0	0	0	0
Lax-Wendroff	1	$\frac{-1}{\tau} + \frac{c^2 \tau}{L^2}$	0	$\frac{(1-\sigma)c}{2b}$	$\frac{-(1+\sigma)c}{2h}$	0	0	0	0
Crank-Nicolson	$\frac{1}{\tau} + \frac{c}{h^2}$	$\frac{\frac{1}{\tau}}{\tau} + \frac{\frac{n^{2}}{c}}{h^{2}}$	0	$\frac{\frac{2\pi}{-c}}{h^2}$	$\frac{\frac{2n}{-c}}{h^2}$	0	$\frac{-c}{h^2}$	$\frac{-c}{h^2}$	0

2. The Sylvester equation.

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

$$(2.1) U = [u_i^n]_{1 \le i \le n_x - 1, 1 \le n \le n_t}$$

Theorem 2.1. The problem (1.2) can be written under the following matricial form:

$$(2.2) M_1 U + U M_2 + \mathcal{L}(U) = M_0$$

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

$$(2.3) \quad M_{1} = \begin{pmatrix} \beta & \delta & 0 & \dots & 0 \\ \varepsilon & \beta & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \beta & \delta \\ 0 & \dots & 0 & \varepsilon & \beta \end{pmatrix} \qquad M_{2} = \begin{pmatrix} 0 & \gamma & 0 & \dots & 0 \\ \alpha & 0 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \gamma \\ 0 & \dots & 0 & \alpha & 0 \end{pmatrix}$$

the matrix M_0 being given by:

$$M_{0} = \begin{pmatrix} -\gamma u_{1}^{0} - \varepsilon u_{0}^{1} - \eta u_{0}^{0} - \theta u_{0}^{1} & -\varepsilon u_{0}^{2} - \eta u_{0}^{0} - \theta u_{0}^{2} & \dots & -\varepsilon u_{0}^{n_{t}} - \eta u_{0}^{n_{t}-1} - \theta u_{0}^{n_{t}} \\ -\gamma u_{2}^{0} - \eta u_{1}^{0} - \vartheta u_{2}^{0} & 0 & \dots & 0 \end{pmatrix}$$

$$\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -\gamma u_{n_{x}-2}^{0} & 0 & \dots & \vdots & \vdots & \vdots \\ -\gamma u_{n_{x}-1}^{0} - \delta u_{n_{x}}^{1} - \eta u_{n_{x}-1}^{0} - \zeta u_{n_{x}}^{2} - \vartheta u_{n_{x}}^{0} & -\delta u_{n_{x}}^{2} - \vartheta u_{n_{x}}^{1} - \zeta u_{n_{x}}^{3} & \dots & -\delta u_{n_{x}}^{n_{t}} - \eta u_{n_{x}-1}^{n_{t}} - \vartheta u_{n_{x}}^{n_{t}-1} \end{pmatrix}$$

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

$$(2.5) \mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 + \mathcal{L}_4$$

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

$$\mathcal{L}_{1}(U) = \zeta \begin{pmatrix} u_{2}^{2} & u_{2}^{3} & \dots & u_{2}^{n_{t}} & 0 \\ u_{3}^{2} & u_{3}^{3} & \dots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ u_{n_{x}-1}^{2} & u_{n_{x}-1}^{3} & \dots & u_{n_{x}-1}^{n_{t}} & 0 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix} \qquad \mathcal{L}_{2}(U) = \eta \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ 0 & u_{1}^{1} & u_{1}^{2} & \dots & u_{1}^{n_{t}-1} \\ 0 & u_{1}^{0} & u_{1}^{1} & \dots & u_{2}^{n_{t}-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & u_{n_{x}-2}^{1} & u_{n_{x}-2}^{2} & \dots & u_{n_{x}-2}^{n_{t}-1} \end{pmatrix}$$

$$(2.6)$$

$$\mathcal{L}_{3}(U) = \theta \begin{pmatrix} 0 & \dots & \dots & 0 \\ u_{1}^{2} & u_{1}^{3} & \dots & u_{1}^{n_{t}} & 0 \\ u_{2}^{2} & u_{2}^{3} & \dots & u_{2}^{n_{t}} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{n_{x}-2}^{2} & u_{n_{x}-2}^{3} & \dots & u_{n_{x}-2}^{n_{t}} & 0 \end{pmatrix} \qquad \mathcal{L}_{4}(U) = \vartheta \begin{pmatrix} 0 & u_{2}^{1} & u_{2}^{2} & \dots & u_{2}^{n_{t}-1} \\ 0 & u_{3}^{1} & u_{3}^{2} & \dots & u_{3}^{n_{t}-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & u_{n_{x}-1}^{1} & \dots & \dots & u_{n_{x}-1}^{n_{t}-1} \\ 0 & 0 & \dots & \dots & 0 \end{pmatrix}$$

$$(2.7)$$

Proposition 2.2. 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 u_{exact} the exact solution of (1.1). The corresponding matrix U_{exact} will be:

$$(2.8) U_{exact} = [U_{exact_i}^{n}]_{1 < i < n_x, 1 < n < n_t}$$

where:

$$(2.9) U_{exact}{}_{i}^{n} = U_{exact}(x_{i}, t_{n})$$

with $x_i = i dx$, $t_n = n dt$.

DEFINITION 2.3. We will call error matrix the matrix defined by:

$$(2.10) E = U - U_{exact}$$

Let us consider the matrix F defined by:

$$(2.11) F = M_1 U_{exact} + U_{exact} M_2 + \mathcal{L}(U_{exact}) - M_0$$

Proposition 2.4. The error matrix E satisfies:

(2.12)
$$M_1 E + E M_2 + \mathcal{L}(E) = F$$

2.2. The matrix equation.

2.2.1. Theoretical formulation. THEOREM 2.5. Minimizing the error due to the approximation induced by the numerical scheme is equivalent to minimizing the norm of the matrices E satisfying (2.12).

Note: Since the linear matricial operator \mathcal{L} appears only in the Crank-Nicolson 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.

Proposition 2.6.

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

$$(2.13) M_1 E + E M_2 = F$$

which is a specific form of the generalized Sylvester equation:

$$(2.14) AX + BXC = D$$

where A and B are m by m matrices, C and F n by n matrices, and X, a m by n matrix. C has to be a Jordan matrix.

PROPOSITION 2.7. Since the coefficient α never vanishes, the matrix M_2 is inversible.

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:

$$(2.15) A = U^*TU$$

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

(2.16)
$$T = \begin{pmatrix} T_1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & T_i & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & T_p \end{pmatrix}$$

where the block matrices T_i , i = 1, ..., p are given by:

(2.17)
$$\begin{pmatrix} \mathcal{R}e\left[\lambda_{i}\right] & \mathcal{I}m\left[\lambda_{i}\right] \\ -\mathcal{I}m\left[\lambda_{i}\right] & \mathcal{R}e\left[\lambda_{i}\right] \end{pmatrix}$$

 $\mathcal{R}e$ 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 $n_x - 1$ 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 (2.13) 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:

(2.18)
$$B = \begin{pmatrix} 0 & \dots & \dots & 0 & -b_0 \\ 1 & 0 & \dots & \dots & 0 & -b_1 \\ 0 & 1 & 0 & \dots & \vdots & \vdots \\ \vdots & 0 & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & -b_{p-1} \end{pmatrix}$$

These results can be generalized through matrix block decomposition to a block companion form matrix:

(2.19)
$$M_2 = \begin{pmatrix} M_2^{B^1} & 0 & \dots & 0 \\ 0 & M_2^{B^2} & 0 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & M_2^{B^k} \end{pmatrix}$$

the $M_2^{B^p}$, $1 \le p \le k$ 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 . Theorem 2.8. In the specific cases of the Lax and Lax-Wendroff schemes, (2.14) has a unique solution.

Proof. (2.14) has a unique solution if and only if A and B have no common eigenvalues.

The characteristic polynomials P_{M_1} , P_{M_2} of M_1 and M_2 , can be respectively calculated as the determinants of respectively $\frac{n_x-1}{2}$ by $\frac{n_x-1}{2}$, $\frac{n_t}{2}$ by $\frac{n_t}{2}$ diagonal block matrices:

(2.20)
$$P_{M_1}(\lambda) = ((\lambda - \beta)^2 - \delta \varepsilon)^{\frac{n_x - 1}{2}}, P_{M_2}(\lambda) = (\lambda^2 - \alpha \gamma)^{\frac{n_t}{2}}$$

In the specific cases of the Lax and Lax-Wendroff schemes: $\alpha \gamma = 0 \neq \pm \beta + \sqrt{\delta \varepsilon}$. Hence, (2.12) has a unique solution, which accounts for the consistency of the given problem.

COROLLARY 2.9. In the specific case of the Leapfrog scheme, (2.14) has a unique solution if and only if $\tau \neq \frac{h}{c}$.

2.3. Specific properties of the matrices M_1 and M_2 .

2.3.1. Inversibility of the matrix M_1 . Theorem 2.10. In the specific case of the Lax and Leapfrog schemes, M_1 is inversible.

THEOREM 2.11. In the specific case of the Lax-Wendroff scheme, M_1 is inversible if and only if

(2.21)
$$\left(\frac{-1}{\tau} + \frac{c^2 \tau}{h^2}\right)^2 \neq \frac{(1 - \sigma^2)c^2}{4h^2}$$

Proof. The determinant D_1 of M_1 can be calculated as the determinant of a $\frac{n_t}{2}$ by $\frac{n_t}{2}$ diagonal block matrix:

$$(2.22) D_1 = (\beta^2 - \delta \varepsilon)^{\frac{n_t}{2}}$$

2.3.2. Nilpotent components of the matrix M_2 . Proposition 2.12. M_2 can be written as:

$$(2.23) M_2 = \alpha^T N + \gamma N$$

where N is the nilpotent matrix, ^{T}N denoting the corresponding transposed matrix:

(2.24)
$$N = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \vdots & \vdots & \dots & 0 & 1 \\ 0 & 0 & \dots & \dots & 0 \end{pmatrix}$$

Proposition 2.13.

For either $\alpha = 0$, or $\gamma = 0$, M_2 will thus be nilpotent, of order n_t .

Proposition 2.14.

For $\gamma = 0$, if M_1 is inversible, the solution at $t = n_t dt$ can then be immediately determined.

Proof.

In such a case, multiplying (2.2) on the right side by $M_2^{n_t-1}$ leads to:

$$(2.25) M_1 U M_2^{n_t-1} + U M_2 M_2^{n_t} = M_0 M_2^{n_t-1}$$

i. e.:

$$(2.26) M_1 U M_2^{n_t-1} = M_0 M_2^{n_t-1}$$

which leads to:

$$(2.27) U M_2^{n_t-1} = M_1^{-1} M_0 M_2^{n_t-1}$$

Due to:

$$(2.28) M_2^{n_t-1} = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & \vdots & \ddots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}$$

we have:

(2.29)
$$U M_2^{n_t - 1} = \begin{pmatrix} u_{1n_t} & 0 & 0 & \dots & 0 \\ u_{2n_t} & 0 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ u_{n_x n_t} & 0 & \dots & 0 & 0 \end{pmatrix}$$

The solution at $t = n_t dt$ can then be immediately determined.

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- 3. Conclusion. Thanks to the above results, we here propose:
- 1. to solve finite difference problems either through the corresponding Sylvester equation, with the aid of a mathematical software such as Mathematica or Maple;
- 2. to study the intrinsic properties of various schemes through those of the related matrices M_1 and M_2 ;
- 3. 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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