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The optimal explicit unconditionally stable box scheme

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Abstract. The finite difference "box" scheme, (see also [1],[2]), is considered on the simplest possible model of single first order linear hyperbolic equation: $u_t + \mu u_x = 0$ with constant coefficient μ and one space variable. The optimal version of the scheme, which is nonoscilating and unconditionally stable with respect to the initial and boundary conditions, is derived in the class of box schemes of the order at least one. If apropriately iterated, this scheme may be applied to general systems of quasilinear first order hyperbolic equations in one space variable, as an explicit, unconditionally stable solver. For more than one space variable this solver is applicable via splitting (see [3]).

Order. Consider the model equation $u_t + \mu u_x = 0$ with $\mu > 0$, and the following finite difference "box" scheme for this equation:

(1) $$au_{k+1}^{n+1} - bu_k^{n+1} + du_{k+1}^n + cu_k^n = 0$$

where u_k^n have to approximate $u(t_n, x_k)$ with $t_n = n\tau$ and $x_k = kh$, while $\tau > 0$ and $h > 0$ are time and space step respectively.

Put

(2) $$\begin{aligned} a &= c_4 + \lambda\mu d_4, & -b &= c_3 + \lambda\mu d_3, \\ c &= c_1 + \lambda\mu d_1, & d &= c_2 + \lambda\mu d_2, \end{aligned} \qquad \lambda = \frac{\tau}{h}.$$

Assume that the solution $u(t,x)$ is in C^3. Inserting the function u into equation (1) and developing, we get in the standard way:

(3) $$\begin{aligned} &[c_1 + c_2 + c_3 + c_4 + \lambda\mu(d_1 + d_2 + d_3 + d_4)]u + \\ &+h[c_2 + c_4 + \lambda\mu(d_2 + d_4)]u_x + \lambda h[c_3 + c_4 + \lambda\mu(d_3 + d_4)]u_t + \end{aligned}$$

$$+\frac{h^2}{2}[c_2 + c_4 + \lambda\mu(d_2 + d_4)]u_{xx} + \lambda h^2[c_4 + \lambda\mu d_4]u_{xt} +$$
$$+\frac{\lambda^2 h^2}{2}[c_3 + c_4 + \lambda\mu(d_3 + d_4)]u_{tt} = o(h^2).$$

Function u and its derivatives have to be taken in (t_n, x_k). Taking into account the equation and its derivatives:

$$u_t + \mu u_x = 0,$$
$$u_{tx} + \mu u_{xx} = 0,$$
$$u_{tt} + \mu u_{xt} = 0,$$

we can write down the formula (3) using only $u(t_n, x_k)$, $u_x(t_n, x_k)$, and $u_{xx}(t_n, x_k)$:

$$[c_1 + c_2 + c_3 + c_4 + \lambda\mu(d_1 + d_2 + d_3 + d_4)]u(t_n, x_k) +$$
$$+h[c_2 + c_4 + \lambda\mu(-c_3 - c_4 + d_2 + d_4) + \lambda^2\mu^2(-d_3 - d_4)]u_x(t_n, x_k) + \tag{4}$$
$$+h^2[\frac{c_1 + c_4}{2} + \lambda\mu(\frac{d_2 + d_4}{2} - c_4) + \lambda^2\mu^2(\frac{c_3 + c_4}{2} - d_4) +$$
$$+\lambda^3\mu^3(d_3 + d_4)]u_{xx}(t_n, x_k) = o(h^2).$$

In order to obtain the residual in (4) of the form $O(h^2)$ at least, we have to set:

$$\begin{aligned} c_1 + c_2 + c_3 + c_4 &= 0,\\ d_1 + d_2 + d_3 + d_4 &= 0,\\ c_3 + c_4 - d_2 - d_4 &= 0,\\ c_2 + c_4 &= 0,\\ d_3 + d_4 &= 0. \end{aligned} \tag{5}$$

This is a system of five linear algebraic equations with eight unknowns c_1,c_2, c_3, c_4, d_1, d_2, d_3, d_4. We may solve the system (5), expressing c_1, c_2, c_3, d_1, d_3 as functions of d_2, d_4 and c_4. Put

$$v = d_2,$$
$$y = d_4,$$
$$z = c_4;$$

we get:

$$\begin{aligned} c_1 &= z - v - y,\\ c_2 &= -z,\\ c_3 &= -c_1 = v + y - z,\\ d_1 &= -v,\\ d_3 &= -y. \end{aligned} \tag{6}$$

Under the conditions (6) the residual of equation (4) is of the form:

$$h^2\lambda\mu\left[\frac{v+y}{2} - z + \frac{\lambda\mu}{2}(v-y)\right]u_{xx}(t_n, x_k) + o(h^2).$$

Denote:

$$p = z - \frac{v+y}{2} - \frac{\lambda\mu}{2}(v-y);$$

this is *the coefficient of diffusion of the scheme (1)*. Now, the coefficients a, b, c, d of equation (1) are the following:

$$\begin{aligned} a &= z + \lambda\mu y = p + \frac{v+y}{2} + \lambda\mu\frac{v-y}{2} + \lambda\mu y = p + (1+\lambda\mu)\frac{v+y}{2}, \\ -b &= v + y - z - \lambda\mu y = -p + (1+\lambda\mu)\frac{v+y}{2}, \\ c &= z - (v+y) - \lambda\mu v = p - (1+\lambda\mu)\frac{v+y}{2}, \\ d &= -z + \lambda\mu v = -p - (1-\lambda\mu)\frac{v+y}{2}. \end{aligned} \tag{7}$$

As a conclusion, let us formulate the following:

PROPOSITION 1. *The scheme* (1) *with coefficients given by formulae* (7) *is of the order one* (*residual is of the form* $O(h^2)$).

If we put $z = \frac{v+y}{2} + \frac{\lambda\mu}{2}(v-y)$ ($p = 0$, *i.e. the diffusion vanishes!*), *then the scheme (1) is of the order two* (*residual is of the form* $O(h^3)$). ∎

Nonoscillation. We are now interested in another feature of scheme (1): *the property of nonoscillation*. In other words, we desire to make a choice of coefficients in (1), which disable creation of parasite oscilations in a solution of finite difference equation (1). It is well known, that such a parasite oscillations apear often in rapidely varying solutions (noncontinuous data), and that they are even able to destroy this solution completely.

Let us now observe how procedes the operation of solving the equation (1). Assume we know:

- initial conditions $u(0, v)$,
- boundary conditions $u(t_n, 0) = g_n$.

The whole process of solving goes on paralelly to the x-axis from $x = 0$, in the direction of the positive semiaxis. This means, that the equation (1) is solved with respect to the variable u_{k+1}^{n+1}. Observe that remaining variables: u_k^{n+1}, u_{k+1}^n, and u_k^n are known. In other words, the process has *the explicit character*.

Assume that the grid contains M points on the x-axis: $x_1, x_2, x_3, ..., x_M$.

Denote: $U^n = [u_1^n, u_2^n, \dots, u_M^n]^T$,

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -b & a & 0 & 0 & \cdots & 0 & 0 \\ 0 & -b & a & 0 & \cdots & 0 & 0 \\ 0 & 0 & -b & a & \cdots & 0 & 0 \\ \cdots \\ 0 & 0 & 0 & 0 & \cdots & -b & a \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ c & d & 0 & 0 & \cdots & 0 & 0 \\ 0 & c & d & 0 & \cdots & 0 & 0 \\ 0 & 0 & c & d & \cdots & 0 & 0 \\ \cdots \\ 0 & 0 & 0 & 0 & \cdots & c & d \end{bmatrix}, \quad f^{n+1} = \begin{bmatrix} g_{n+1} \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

The scheme (1) can be written as the recurrence formula:

$$AU^{n+1} + BU^n = f^{n+1}$$

or, equivalently,

$$U^{n+1} = CU^n + g^{n+1}, \tag{8}$$

where $C = -A^{-1}B$ and $g^n = A^{-1}f^n$. We can now present the equation (8) in the explicit form:

$$U^n = C^nU^0 + C^{n-1}g^1 + C^{n-2}g^2 + \cdots + C^{n-1}g^{n-1} + g^n. \tag{9}$$

From (9) it is clear, that *nonnegativity of the elements of the matrix C is a sufficient condition for "nonoscillation" in U^n.*

It is easy to compute the elements of C directly:

$$C = -\Big(\sum_{k=0}^{M-1} \gamma^k E^k\Big) diag(1, a, a, \cdots, a)^{-1} B,$$

where $\gamma = \frac{b}{a}$, and E is following nilpotent matrix of the dimension M:

$$E = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots 0 & 0 \\ 1 & 0 & 0 & 0 & \cdots 0 & 0 \\ 0 & 1 & 0 & 0 & \cdots 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots 0 & 0 \\ \cdots \\ 0 & 0 & 0 & 0 & \cdots 1 & 0 \end{bmatrix}.$$

PROPOSITION 2. *If $v + y > 0$, then the following conditions are sufficient for nonoscillation of the scheme* (1):

$$|p| \le (1 + \lambda\mu)\frac{v + y}{2}$$

and

$$(1-\lambda\mu)\frac{v+y}{2}\le p \quad \text{if } \lambda\mu\le 1$$
$$(\lambda\mu-1)\frac{v+y}{2}\le p \quad \text{if } 1<\lambda\mu.$$

The scheme (1) *is optimal (i.e. the coefficient* p *of diffusion is minimal,* $p=|1-\lambda\mu|\frac{v+y}{2}$ *) if*

1. $0<\lambda\mu\le 1$ *and*

$$a=v+y,\qquad b=0,\qquad c=-\lambda\mu(v+y),\qquad d=-(1-\lambda\mu)(v+y)$$

("backward upwind scheme").

2. $\lambda\mu>1$ *and*

$$a=\lambda\mu(v+y),\qquad b=(\lambda\mu-1)(v+y),\qquad c=-(v+y),\qquad d=0$$

(a kind of "implicit backward Euler scheme").

Proof. A sufficient condition for nonoscilation is the positivity of all the elements of the matrix C. Since $\lambda\mu>0$, this last condition is satisfied if the following tree inequalities hold:

$$\begin{aligned} a&=p+(1+\lambda\mu)\frac{v+y}{2}\ge 0,\\ b&=p-(1-\lambda\mu)\frac{v+y}{2}\ge 0,\\ c&=p-(1+\lambda\mu)\frac{v+y}{2}\le 0,\\ -d&=p+(1-\lambda\mu)\frac{v+y}{2}\ge 0. \end{aligned}\tag{10}$$

The inequqlity $|p|\le(1+\lambda\mu)\frac{v+y}{2}$ implies directly $a\ge 0$ and $c\le 0$.

If $\lambda\mu\le 1$, then $0\le p-(1-\lambda\mu)\frac{v+y}{2}=b$ and $-d=p+(1-\lambda\mu)\frac{v+y}{2}\ge p-(1-\lambda\mu)\frac{v+y}{2}=b\ge 0$.

If $\lambda\mu>1$ then $0\le p-(\lambda\mu-1)\frac{v+y}{2}=p+(1-\lambda\mu)\frac{v+y}{2}=-d$ and $b=p+(\lambda\mu-1)\frac{v+y}{2}\ge p-(\lambda\mu-1)\frac{v+y}{2}=-d\ge 0$. ∎

Stability. Let us now investigate the stability of the scheme (1). We shall consider separately the stability with respect to the initial and the boundary conditions, using the so called Fourier Method.

1. Stability with respect to the initial conditions. We shall look for the solution of the form

$$u_k^n=\gamma^n e^{i\alpha k},$$

where α is an arbitrary real number and γ is complex. Inserting u_k^n into (1), we get the following formula for the absolute value of γ:

$$|\gamma|^2 = \frac{c^2 + d^2 + 2cds}{a^2 + b^2 - 2abs},$$

where $s = \cos\alpha$, hence s is an arbitrary real number such that $-1 \leq s \leq 1$. Let $q = z - v - y$; then

$$\Phi(s) = |\gamma|^2$$
$$= \frac{q^2 + z^2 - 2v\lambda\mu(q+z) + 2v^2\lambda^2\mu^2 - 2s(qz - v\lambda\mu(q+z) + v^2\lambda^2\mu^2)}{q^2 + z^2 + 2y\lambda\mu(q+z) + 2y^2\lambda^2\mu^2 - 2s(qz + y\lambda\mu(q+z) + y^2\lambda^2\mu^2)}.$$

Observe that the first derivative $\Phi'(s)$ is of the constant sign in any interval of its domain, hence $\Phi(s)$ assumes its global maximum in the interval $[-1, 1]$ for $s = -1$ or $s = 1$. We have:

$$\Phi(-1) = \frac{(q+z)^2 + 4v^2\lambda^2\mu^2}{(q+z)^2 + 4y\lambda\mu(q+z) + 4y^2\lambda^2\mu^2},$$
$$\Phi(1) = 1.$$

The scheme (1) is stable if $\Phi(-1) \leq 1$ or, equivalently, if

$$v^2\lambda\mu \leq y(q+z) + y^2\lambda\mu. \tag{11}$$

According to the definition of the coefficient p of diffusion, we may write:

$$\frac{q+z}{2} = z - \frac{v+y}{2} = p + \frac{\lambda\mu}{2}(v-y).$$

Expressing now p in the form

$$p = |1 - \lambda\mu|\frac{v+y}{2}r$$

with nonnegative parameter r, we get another form of the inequality (11):

$$v^2\frac{\lambda\mu}{2} \leq \left[|1-\lambda\mu|\frac{v+y}{2}r + \frac{\lambda\mu}{2}(v-y)\right] + y^2\frac{\lambda\mu}{2}.$$

Put $\omega = \frac{v}{y}$ and multiply the last inequality by $\frac{2}{y^2}$; we get the equivalent inequality

$$\lambda\mu\omega^2 - (|1-\lambda\mu|r + \lambda\mu)\omega - |1-\lambda\mu|r \leq 0. \tag{12}$$

It is easy to verify that the binomial at the left hand side of the inequality (12) has two real roots: $\omega_1 \leq 0$ and $\omega_2 \geq 1$, hence the final version of the stability condition has the form:

$$\omega_1 \leq \omega \leq \omega_2.$$

Hence, we have always stability with respect to the initial condition if $0 < v \leq y$. We can now formulate:

PROPOSITION 3. *If $0 < v \leq y$ and $r \geq 0$, then the scheme (1) with coefficients given by formulae (7) is stable with respect to the initial condition.*

Remark. If $r = 0$, then the scheme (1) is of the order two. If $1 \leq r \leq \frac{|1+\lambda\mu|}{|1-\lambda\mu|}$, then the scheme (1) is nonoscillating.

2. Stability with respect to the boundary condition. Now, we are looking for the particular solution of the equation (1), of the form:

$$u_k^n = \gamma^k e^{i\alpha n},$$

where α is an arbitrary real number and γ is complex. Inserting u_k^n into equation (1) we get the following formula for $|\gamma|$:

$$\Phi(s) = |\gamma|^2 = \frac{b^2 + c^2 - 2bcs}{a^2 + d^2 + 2ads},$$

where $s = \cos\alpha$. Since, again, the first derivative of the function Φ is of the constant sign, it is enough to consider only $\Phi(-1)$ and $\Phi(1)$. Using the formulae (7) we get:

$$\Phi(-1) = \frac{4p^2 + (v+y)^2 - 4p(v+y)}{4p^2 + (v+y)^2 + 4p(v+y)},$$

$$\Phi(1) = \frac{[\lambda\mu(v+y)]^2}{[\lambda\mu(v+y)]^2} = 1.$$

We obtain the following

PROPOSITION 4. *The scheme (1) with coefficients given by the formulae (7) is stable with respect to the boundary condition if:*

$$p \geq 0$$

and

$$v + y \geq 0.$$

Remark. The choice $p \geq 0$ (as suggested by the Proposition 4), and $v = y$ is always good; since the scheme (1) depends in fact on $v + y$, we may always put $v + y = 1$. This choice gives a simple form of the optimal schemes of the Proposition 2:

1. $0 < \lambda\mu \leq 1$ and

$$a = 1, \qquad b = 0, \qquad c = -\lambda\mu, \qquad d = \lambda\mu - 1,$$

2. $\lambda\mu > 1$ and

$$a = \lambda\mu, \qquad b = \lambda\mu - 1, \qquad c = -1, \qquad d = 0.$$

A general remark on stability. Let us apply scheme (1) on the rectangular grid with steps $h > 0$ and $\tau > 0$ (on the x and t axes respectively) to the following model initial - boundary value problem:

$$(11)\qquad \begin{aligned} u_t + \mu u_x &= 0, & \mu &> 0,\\ u(0,x) &= \Phi(x), & 0 \le x &\le L,\\ u(t,0) &= \Psi(t), & 0 \le t &\le T. \end{aligned}$$

According to the CFL condition, the strip of the plane:

$$0 \le x \le L,$$
$$0 \le t \le T$$

is divided into two disjoint domains of influence by the stright line $t = \lambda x$, where $\lambda = \frac{\tau}{h}$. The part under this stright line is uniquely influenced by the initial condition, while the part over the stright line, by the boundary condition. This observation justifies our technique of treating separately the stability with respect to the initial and the boundary conditions, at least on the discussed model problem.

Numerical experiments. The program which computes the solution of the model problem (13) applies in general the "classical box scheme" with zero diffusion ($p = 0$). If, however, the sudden jump of the deivative of the solution or quick oscillations appear, then the classical box scheme is replaced by the optimal one, according to Proposition 2. The decision concerning the local choice of the scheme depends on parameters defining the upper bound of the the derivative of the solution and the upper bound of the oscillation of the solution, wich are considered as admissible for the classical box scheme. These two parameters are among the data of the program.

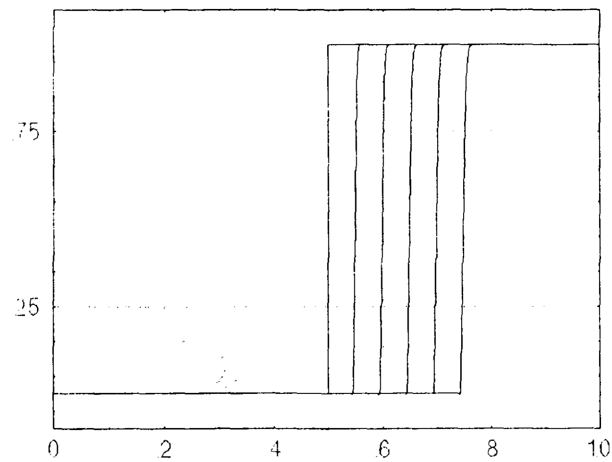

Figure 1. Evolution of the step-function from the left to the right: numerical solution of the equation $u_t + u_x = 0$; space step $h = .002$, time step $\tau = .001$, number of steps: 250

References

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