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ON MONOTONE DIFFERENCE SCHEMES FOR WEAKLY COUPLED SYSTEMS OF PARTIAL DIFFERENTIAL EQUATIONS

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1. Formulation of the problem

We consider here systems of partial differential equations of mixed type,

$$(1) \qquad C\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(A\frac{\partial u}{\partial x}\right) + B\frac{\partial u}{\partial x} - Du + f, \qquad 0 < x < 1, \ 0 < t \leqslant T,$$

where u and f are p-vectors, and C, A and B are diagonal $p \times p$ matrices, respectively, with elements c_k , a_k and b_k . The equations (1) are coupled only through $D = (d_{kl})$ which may be a full matrix. All functions depend smoothly on x and t. Moreover, we assume the inequalities

$$(*) c_k, a_k \geqslant 0, d_{kk} \geqslant -\sum_{\substack{l \neq k \\ k,l=1,\ldots,p}} d_{kl}, d_{kl} \leqslant 0, k \neq l,$$

to hold. Along with (1) there are given boundary conditions of first, second or third kind,

$$\begin{vmatrix} (2.1) & u_k \\ (2.2) & -a_k \frac{\partial u_k}{\partial x} \\ (2.3) & -a_k \frac{\partial u_k}{\partial x} + \varkappa_k^0 u_k \end{vmatrix} = v_k^0(t), \ x = 0, \quad a_k \frac{\partial u_k}{\partial x} \\ a_k \frac{\partial u_k}{\partial x} + \varkappa_k^1 u_k \end{vmatrix} = v_k^1(t), \ x = 1,$$

(the type of the boundary conditions may vary with k, x and t) and initial conditions

(3)
$$u(x, 0) = u_0(x), \quad 0 \le x \le 1.$$

The boundary value problem (1)-(3) serves to model a great variety of processes in chemics, biology, agriculture, water research and physics, see, e.g., [1]-[5]. Often there are nonlinearities in the right-hand sides functions. Then, (1)-(3) is the problem to be solved in every step of a Newton iteration. For this subject, see [6].

2. Numerical questions connected with (1)-(3)

In the applications, the relations (*) often take place. For example, in chemical problems, (*) is found to hold if u represents the vector of the concentrations of appropriately chosen independent components of the reaction.

If the relations (*) are sharpened somewhat $(c_k, a_k \geqslant c_0 > 0$, some condition excluding a zero eigenvalue in the case of second boundary conditions), the maximum principle is known to hold, see [7], p. 190. The maximum principle and its consequences express important physical properties (domination of the values of state parameters by their values on the boundary, preservation of positiveness and monotonicity). Therefore, we are interested in discrete models of (1)–(3) which share with that system those properties. Hence, for the numerical solution of (1)–(3) we shall consider below a difference scheme which has, regardless of the discretization, the property to be monotone, that is, to fulfil the conditions of the maximum principle (see, e.g., [8], p. 245).

For the usual difference schemes (for instance, if the first derivatives $b_k \frac{\partial u_k}{\partial x}$ in (1) are approximated by central differences) the conditions of the maximum principle are fulfilled not in general but under restrictions like $|b_k h/2a_k| \leq 1$, h being the spatial discretization step. In problems with strong convection and small diffusion (a frequent situation) this is a cumbersome condition. To get stability, the first derivatives are often approximated by one-sided differences ("upstream differencing"), but this introduces an additional (numerical) diffusion of the magnitude $|b_k h/2|$. The same is true for the scheme [8], p. 432.

Another approach has been given in [9] where for the case of a scalar equation (1) with D=0 a difference scheme is constructed which is monotone for any discretization (h, τ) , τ the time step and h the possibly nonequidistant spatial step. The scheme [9] approaches the method of characteristics if $A \rightarrow 0$ and $|B\tau/Ch| \rightarrow 1$. This property allows (by appropriate choice of h and τ) for a reduction of the numerical diffusion which becomes drastical for coefficients depending on x only.

The idea of [9] has been developed further in [10] and [11] to cover the case $D \neq 0$. Practically (see the computational results in [10]), the

construction of a difference scheme has been accomplished which is maximum norm stable for any discretization if (*) is satisfied. All coefficients may degenerate, even jointly (if only there remains an equation determining u), and in whole subintervals. Theoretically, A+C>0 is sufficient (pointwise) to satisfy the conditions of the maximum principle, and $C \geqslant C_0 > 0$ (and some restriction on the possibility to pose second kind boundary conditions) is sufficient to prove maximum norm stability.

In this paper, the scheme [11] is applied to (1)-(3), and numerical results are given for systems with constant coefficients. Moreover, an idea of [12] is used to construct a difference scheme which is maximum norm stable for a certain class of nonlinear right-hand sides f.

Difference schemes for solution of systems like (1)-(3) have also been considered in [8], p. 504, [15]-[18] (and in further papers cited there), but those schemes, even if constrained to one dimension in space, are monotone not for any coefficients satisfying (*) and not for any discretization.

3. Notations

We need the following notations (essentially, those of [8]): Let $\omega_h := \{x_i, i = 1, ..., N-1\}$ be the nonequidistant spatial grid with $h_{i-1/2} := x_i - x_{i-1} > 0$, $x_0 := 0$, $x_N := 1$, $\overline{\omega}_h := \omega_h \cup \{x_0, x_N\}$. We put $y(x_i) = y_i$, $y_{i \pm 1/2} := y(x_i \pm h_{i \pm 1/2})$, and these notations are also used for expressions containing grid functions. The forward and backward differences are

$$y_{x,i} := (y_{i+1} - y_i)/h_{i+1/2}, \quad y_{\overline{x},i} := (y_i - y_{i-1})/h_{i-1/2}.$$

With respect to t we have the nonequidistant grid $\omega_{\tau} := \{t_j, j=0, ..., m-1\}$, $\tau := t_{j+1} - t_j > 0$, $t_0 := 0$, $t_m := T$, and we use the notations $y^j := y(t_j), \ y^{j+1/2} := y(t_j + \tau/2), \ y^{(\sigma)} := \sigma y^{j+1} + (1-\sigma)y^j$, and $y_t := (y^{j+1} - y^j)/\tau$. (The time step τ is not indexed since we are considering two-level difference schemes only.)

4. The formulae of the difference scheme

Our difference scheme belongs to the three-point, two-level schemes and is defined by the following formulae which constitute the adaption of [11] to the weakly coupled system (1):

$$(4) \qquad \overline{h}M_{a}^{\sigma}(c_{k})(y_{k})_{t} = \overline{h}A_{a}^{\sigma}(a_{k}, b_{k})y_{k} - \overline{h}\sum_{l=1}^{p}H_{a}^{\lambda,\mu,\nu}(d_{kl})y_{l} + \overline{h}M_{a}f_{k}^{(\sigma)},$$

$$k = 1, \ldots, p, \ t \in \omega_{\tau},$$

$$x \in \begin{cases} \omega_{h} & \text{first} \\ \text{in case of} & \text{kind boundary values.} \\ \overline{\omega}_{h} & \text{second} \end{cases}$$

Here

$$a = a(q), \quad q = q_k := \begin{cases} b_k h/2a_k, & a_k + |b_k| > 0, \\ 0, & a_k = b_k = 0, \end{cases}$$

$$(5) \quad a(z) := (\varrho(z) - 1)/2z,$$

$$\rho(z) := z \coth z \quad \text{or} \quad \varrho(z) := (3 + 3|z| + 3z^2 + 2|z|^3)/(3 + 3|z| + 2z^2).$$

The following definitions hold for $x = x_i \in \omega_h$ (excluding the special case $a_{i\pm 1/2} = 0$, $b_{i+1/2} < 0$, $b_{i-1/2} > 0$ considered later):

$$\begin{split} (\overline{h}M_{a}^{\sigma}(c)y_{t})_{i} &:= 2\left(\sigma c h \max(0, a)\right)_{i+1/2}y_{t,i+1} +\\ &+ \left[\left(c h\left(\frac{1}{2} + a - 2\sigma \max(0, a)\right)\right)_{i+1/2} + \left(c h\left(\frac{1}{2} - a - 2\sigma \max(0, a)\right)\right)_{i-1/2}\right]y_{t,i} +\\ &+ 2\left(\sigma c h \max(0, -a)\right)_{i-1/2}y_{t,i-1},\\ &(\overline{h}A_{a}^{\sigma}(a, b)y)_{i} := \left(a + b h\left(\frac{1}{2} + a\right)\right)_{i+1/2}y_{x,i}^{(\sigma_{i+1/2})} - \left(a - b h\left(\frac{1}{2} - a\right)\right)_{i-1/2}y_{\overline{x},i}^{(\sigma_{i-1/2})},\\ &(\overline{h}H_{a}^{\lambda,\mu,\nu}(d)y)_{i} \\ &:= 2\left(\lambda d h \max(0, a)\right)_{i+1/2}y_{i+1}^{(\mu_{i+1/2})} + \left(d h\left(\frac{1}{2} + a - 2\lambda \max(0, a)\right)\right)_{i+1/2}y_{i}^{(\nu_{i+1/2})} +\\ &+ \left(d h\left(\frac{1}{2} - a - 2\lambda \max(0, -a)\right)\right)_{i-1/2}y_{i}^{(\nu_{i-1/2})} + 2\left(\lambda d h \max(0, -a)\right)_{i-1/2}y_{i-1}^{(\mu_{i-1/2})},\\ &(\overline{h}M_{a}f_{k}^{(\sigma)})_{i} := \left(h f_{k}^{(\sigma)}\left(\frac{1}{2} + a\right)\right)_{i+1/2} + \left(h f_{k}^{(\sigma)}\left(\frac{1}{2} - a\right)\right)_{i-1/2}. \end{split}$$

Here σ , λ , μ , ν are weighting parameters determined below in Section 6; their dependence on k is not indicated. These parameters, as well as all coefficients, are taken at the grid midpoints $(x_{i+1/2}, t_{i+1/2})$.

For $a_{i+1/2} = 0$, $b_{i+1/2} < 0$, $b_{i-1/2} > 0$, $x \in \omega_h$, we use the definitions

$$\begin{split} & \big(\overline{h} M_{a}^{\sigma}(c) y_{i} \big)_{i} := \frac{1}{2} \big[(ch)_{i+1/2} + (ch)_{i-1/2} \big] y_{t,i}, \\ & \big(\overline{h} A_{a}^{\sigma}(a,b) y \big)_{i} := 0, \\ & \big(\overline{h} H_{a}^{\prime,\mu,\nu}(d) y \big)_{i} := \frac{1}{2} \big[(dh)_{i+1/2} + (dh)_{i-1/2} \big] y_{i}^{(\nu_{i})}, \\ & (\overline{h} M_{a} f_{k}^{(\sigma)})_{i} := \frac{1}{2} \big[(hf_{k})_{i+1/2} + (hf_{k})_{i-1/2} \big]^{(\sigma_{i})}, \end{split}$$

that is, formally we put $b_{i\pm 1/2}=0$ in the earlier definitions. Note, that the weighting parameters are taken here at $(x_i,\,t_{j+1/2})$.

5. The boundary conditions

For the boundary conditions (2.1) we put, as usual,

$$(y_k)_0^{j+1} = (v_k^0)^{j+1}, \quad (y_k)_N^{j+1} = (v_k^1)^{j+1}.$$

The approximation of (2.2) is given by (4) where all nondefined symmetric symmetric symmetric symmetric symmetric symmetric bols (those indexed -1, -1/2, N+1/2, N+1) have to be deleted and

 $(\nu_k^0)^{(\sigma_{1/2})}$, $(\nu_k^1)^{(\sigma_{N-1/2})}$ are added to $(hf_k^{(\sigma)}(\frac{1}{2}+a))_{1/2}$, $(hf_k^{(\sigma)}(\frac{1}{2}-a))_{N-1/2}$, respectively. In this way natural difference boundary conditions are obtained. Such boundary conditions are advantageous with respect to conservativity: they close the "discrete conservation law" obtained by summing up the equations (4) over $\overline{\omega}_h$.

Similarly, (2.3) is approximated by taking the natural difference boundary conditions and adding $-\varkappa_k^0(y_k)_0$ and $-\varkappa_k^1(y_k)_N$ to $(\bar{h}\Lambda_a^\sigma(a_k,b_k)y_k)_i$, i=0,N, respectively.

To be sure of the unique solvability of the equations (4), the boundary conditions must be posed properly:

- (a) Second kind conditions must not be posed in boundary points $(x_i, t_{j+1/2}), i = 0, N$, where $a_{1/2} = 0, b_{1/2} < 0$ or $a_{N-1/2} = 0, b_{N-1/2} > 0$, respectively.
- (b) If $c_{i+1/2} = d_{i+1/2} = 0$ for some $t = t_{j+1/2}$ and all i, then second kind conditions must not be posed in at least one of the points (x_0, t_{j+1}) and (x_N, t_{j+1}) .

6. The weighting parameters

We restate now from [11] the definition of the weighting parameters σ , λ , μ , ν guaranteeing the maximum principle. In [10] it has been explained how to get these conditions which are pointwise ones and do not interconnect values of the coefficients at neighbouring points.

We remark that the weighting parameters are not determined uniquely by the conditions of the maximum principle. A certain freedom exists which has been used to diminish the magnitude of the artificial distributed sources introduced by the difference scheme. There are no such sources, i.e. the scheme is conservative, in the Crank-Nicolson case $\sigma \equiv \lambda \equiv \mu \equiv \nu \equiv \frac{1}{2}$, and it showed to be possible to select the weighting parameters in such a way that quite frequently there holds $\sigma = \mu = \nu$, $\lambda = \frac{1}{2}$.

Below, in the formulae defining the weighting parameters, we have adopted the following notations: The equation number k is omitted. All symbols without an index are to be taken at $(x_{i-1/2}, t_{j+1/2})$. If α occurs without argument then it is (only in this section) equal to $|\alpha(q)|$, see (5). Finally,

$$r = d\tau/2c$$
, $A = (a/h + |b|(\frac{1}{2} + a))\tau/ch$, $d = d_{kk}$.

(a) special cases:

(a1) if
$$a_{i\pm 1/2}=0$$
, $b_{i+1/2}<0$, $b_{i-1/2}>0$, then we take

$$\sigma_i = v_i = \frac{1}{2} + \alpha(\bar{r}_i), \quad \bar{r}_i := \tau[(dh)_{i+1/2} + (dh)_{i-1/2}]/2[(ch)_{i+1/2} + (ch)_{i-1/2}],$$

(a2) if
$$c = 0$$
, then
$$\sigma = \nu = \mu = 1, \quad \lambda = \min(\frac{1}{2}, (a/h + |b|(\frac{1}{2} + a))/2ahd);$$
(b) if the special cases do not apply: (b1) if $A < 2a$ then we take $\sigma = \lambda = 0$, if $A = 2a$ then $\sigma = \frac{1}{2} + a(r), \lambda = \frac{1}{2} - a(r),$ and in both cases
$$\mu = 0, \quad \nu = \max(\sigma, 1 - (\frac{1}{2} + a - A)/2r(\frac{1}{2} + (\frac{1}{2} - \lambda)2a));$$
(b2) if $A > 2a$ then
$$\sigma = \max(\frac{1}{2} + a(r), 1 - (\frac{1}{2} - a)/(A - 2a + 2r(\frac{1}{2} + a))),$$

$$\mu = \min(\sigma, (A - 2a)/4ra), \quad \nu = \max(\sigma, 1 - 1/2r),$$

$$\lambda = \min(\frac{1}{2}, ((1 - \sigma)A + 2a\sigma)/4r(1 - \mu)a).$$

That the weighting parameters are the same for the system (1) as for one equation [11] is a consequence of the assumption (*) on the isotonicity of the matrix D.

7. Maximum norm stability

Similarly as in [10], we are sure to have the maximum principle for the difference scheme (4) if the following conditions are satisfied: The assumptions (*) are true, the boundary conditions (2) are posed properly, the weighting parameters are selected as described in Section 6, and $a_k + c_k > 0$ holds pointwise for all k. For $c_k \ge c_0 > 0$, all k, we can obtain an estimate showing the maximum norm stability of (4).

For one scalar equation (1) in [10] there has been given a numerical example where first order accuracy was observed without c > 0 or a + c > 0 taking place.

8. On the natural difference boundary conditions

We shall show now on two examples that the natural difference boundary conditions are very useful if the diffusion coefficient is identically zero or degenerates in a strip containing the boundary, and hence boundary conditions must not been posed on one or both sides of the *x*-interval. This is true for the problem (1)–(3), but in the difference formulation conditions are needed to close the system of equations or to get values of the solution also on the boundary. In such cases now, the natural difference boundary conditions with $\nu^0(t) \equiv \nu^1(t) \equiv 0$ do what is required:

- (a) Let be $a_k = 0$, and c_k , $b_k > 0$. Then in the continuous formulation there are no conditions for y_k at x = 0. By definition, the natural difference boundary conditions at x = 0 are obtained from (4) by putting i = 0 and deleting all expressions indexed -1 or -1/2. It is checked immediately that for i > 0 the corresponding expressions (indexed i-1, i-1/2) are zero due to a = 1/2, see (5). Hence, we have just what is needed: The boundary condition turns out to be an approximation of the differential equation itself, moreover, it is the same approximation as used in the inner of the x-interval.
- (b) Let be $a_k = b_k = 0$, but $c_k > 0$. Hence, the problem (1)-(3) does not contain boundary conditions for y_k neither at x = 0 nor at x = 1. By definition, a = 0. Then, the difference operators in (4) are given by the same formulae as written out for the special case $a_{i\pm 1/2} = 0$, $b_{i+1/2} < 0$, $b_{i-1/2} > 0$. From there the natural difference boundary conditions are readily obtained: they constitute, essentially, the same difference scheme as taken in inner points, up to the factor 1/2 (in correspondence with the trapezoid rule).

9. Some numerical results

Firstly, we give results for systems (1)-(3) of two equations with constant coefficients. Here, right-hand sides, first kind boundary values and initial data were fitted to the exact solution $u = (1+xt, 1+xt+x^2)$, the time interval was (0, 0.1], the spatial grid equidistant with h = 1/40.

(a) Coupling of a hyperbolic and an elliptic equation:

$$C = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} 1 & -1/2 \\ -1 & 1 \end{bmatrix}.$$

For the hyperbolic equation, in accordance with Section 8, natural difference boundary conditions were posed at x=1. The maximum norm error e_k in the calculation of u_k by the difference scheme (4) with $\tau=1/40$ was found to be

$$e_1 = 2.807 - 5$$
, $e_2 = 5.484 - 6$.

(b) Coupling of a parabolic and an ordinary (in x) differential equation:

$$A = \begin{bmatrix} 0.01 & 0 \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad \text{the matrices } C \text{ and } D \text{ are the same}$$
 as in (a).

For the ordinary differential equation natural difference boundary conditions were posed at x = 0. Results:

$$e_1 = 1.264 - 5$$
, $e_2 = 2.775 - 4$.

(c) A system of two elliptic equations:

C=0, B=0, the matrices A and D are the same as in (b).

Results obtained after the one necessary "time" step:

$$e_1 = 8.285 - 6$$
, $e_2 = 2.754 - 5$.

Using the program written especially for solution of systems (1)–(3) of two equations with constant coefficients, several problems from chemics and agriculture (including coupling of parabolic and hyperbolic resp. ordinary (in t) differential equations) have been solved. Due to the small computing times (on a grid of 40×100 points 5.8 seconds of CPU time were needed on a machine with 10^5 operations per second) it was possible to determine parameters in the differential equations from measurement data. The systems of blocktridiagonal equations resulting from the difference scheme have been solved by the well-known algorithm of specialized Gauß elimination, see [13], [14], p. 106, and [19].

For the general case (1)-(3) a program has been written which admits dependence of the coefficients on x, t, u and $\partial u/\partial x$. The nonlinearities are tried to solve by simple iteration. In an academic example with h=1/80, p=4, $c_k=1+k^3$, $a_k=10^k$, $b_k=0$, $d_{kk}=10^{4-k}$, $d_{kl}=0$, k>l, $d_{kl}=-d_{kk}\cdot 2^{k-l}$, k<l, with right-hand sides f, first kind boundary data and initial values fitted to the exact solution $u_k=\cos t \sin kx$, after 20 steps using $\tau=1/20$ the following results were obtained:

$$e_1 = 2.606 - 4$$
, $e_2 = 3.637 - 4$, $e_3 = 2.698 - 4$, $e_4 = 1.514 - 5$, CPU time: 63 sec.

The program was used to solve problems from chemical engineering, and showed to work very effectively.

10. A monotone difference scheme for systems with nonlinear sources

We rewrite now -Du+f in (1) as -f(u, x, t) and use the idea of [12] to construct a scheme which is maximum norm stable for mappings f of the p-dimensional Euclidean space into itself being monotone in the sense of [20],

$$(f(u-v), u-v) = \sum_{k=1}^{p} f_k(u-v, x, t)(u_k-v_k) \geqslant 0,$$

and satisfying, moreover,

$$f(0,x,t)=0.$$

The coefficients c, a, b are assumed to be the same for all equations of (1), i.e. they do not depend on k.

We define now

$$(Ay)_i := (a + bh(\frac{1}{2} + a))_{i+1/2} y_{x,i} - (a - bh(\frac{1}{2} - a))_{i-1/2} y_{x,i}^{-1}$$

where a is given by (5).

Then the difference scheme is

(6)
$$ch(y_k)_t = Ay_k^{j+1} - hf_k(y^{j+1}), \quad x \in \omega_h, \ t \in \omega_\tau,$$

where

$$ch = (ch)_i := \frac{1}{2}[(ch)_{i+1/2} + (ch)_{i-1/2}], \quad h = h_i := \frac{1}{2}(h_{i+1/2} + h_{i-1/2}).$$

Using the identities

$$\begin{split} 2y^{j+1}y_t &= (y^2)_t + \tau(y_t)^2, \qquad 2yy_x &= (y^2)_x - h_{i+1/2}(y_x)^2, \\ 2yy_x^- &= (y^2)_x^- - h_{i-1/2}(y_x^-)^2, \end{split}$$

we get from (6) by multiplying with $2y_k^{j+1}$

$$\begin{split} ch\left[(y_k^2)_t + \tau\left((y_k)_t\right)^2\right] &= \left(a + bh\left(\frac{1}{2} + a\right)\right)_{i+1/2} \left[(y_k^2)_x - h_{i+1/2}\left((y_k)_{x,i}\right)^2\right] - \\ &- \left(a - bh\left(\frac{1}{2} - a\right)\right)_{i-1/2} \left[(y_k^2)_x + h_{i-1/2}\left((y_k)_{x,i}\right)^2\right] - \\ &- y_k^{j+1} f_k(y^{j+1}, x, t)h. \end{split}$$

After summing up these equations with respect to k and introducing $z = \sum_{k=1}^{p} y_k^2$, we find

$$chz_{t} = Az^{j+1} - R,$$

where

(8)
$$R := (f(y^{j+1}), y^{j+1}) + \sum_{k=1}^{p} \{ [(a + bh(\frac{1}{2} + a))h]_{i+1/2} ((y_k)_{x,i})^2 + [(a - bh(\frac{1}{2} - a))h]_{i-1/2} ((y_k)_{x,i})^2 + ch\tau((y_k)_t)^2 \} \ge 0$$

due to the assumptions on f and the definition of a which implies $a \pm bh(\frac{1}{2} \pm a) \ge 0$. From (7) and (8) it follows by the maximum principle that z takes on its maximum on the boundary. Hence, $|y_k|$ is estimated by the maximum of the Euclidean norm of the boundary and initial values, which shows the maximum norm stability of (6). Unicity of the solution of (6) is also a consequence of the monotonicity of f. Another question

is, of course, how to obtain that solution. In the case f(u, x, t) = Du with a nonnegative matrix D = D(x, t) the shortened Gauß elimination is used once more. In the nonlinear case the Newton method may be applied, cf. [6], which in every step leads to linear systems with a nonnegative coupling matrix.

To finish, we mention that in the above consideration first kind boundary conditions have been assumed tacitly. However, the same approach works for second and third kind boundary conditions approximated analogously as described in Section 5.

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