# NONNEGATIVITY OF THE NUMERICAL SOLUTION OF PARABOLIC PROBLEMS WITH DIFFERENT BOUNDARY CONDITIONS

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#### 1. Introduction

In this paper we study the nonnegativity of the numerical solution of the parabolic problems with second and third boundary conditions in one-dimensional case. Using the FEM's linear basis functions for the space-discretization and the single-step method for the time discretization we formulate a new sufficient condition for the time step which guarantees the nonnegativity of the numerical scheme.

#### 2. Formulation of the problem

We shall consider the liner parabolic problem in one dimension having the form

(2.1) 
$$\frac{\partial U}{\partial t} - \frac{\partial^2 U}{\partial x^2} = F(x, t); \quad 0 < x < L; \quad t > 0,$$

(2.2) 
$$U(x,t) = u_0(x); \quad 0 \le x \le L,$$

(2.3) 
$$U(0,t) = \frac{\partial U}{\partial x}(L,t) = 0; \quad t > 0.$$

It is well known [6] that under some natural conditions (it means that the initial function  $u_0$  and the source function F are sufficiently smooth and nonnegative) the problem (2.1)-(2.3) has a nonnegative solution on the whole domain  $G = [0, L] \times R$  [6]. This property plays an important part in applications.

E.g. if (2.1)-(2.3) describes the process of heat conduction then the boundary conditions (2.3) mean the following: at the point x = 0 the temperature is given and at the point x = L there is heat isolation. Our main goal is to examine the condition of the nonnegativity of the numerical solution when we apply the Galerkin method with linear basis functions to the semidiscretization and the single-step method to the solution of the ODE's system [3]. For the sake of simplicity we consider the problem (2.1)-(2.3) without the source function, that is F = 0. We seek the numerical solution in the form

(2.4) 
$$U_h(x,t) = \sum_{i=1}^n \alpha_i(t)\phi_i(x),$$

where n is the number of the intervals and  $\phi_i(x)$  are piecewise linear functions with equidistant spaced nodes  $x_i = ih$ , defined by

$$\phi_i(x) = \begin{cases} \frac{x - h(i-1)}{h} & ; & h(i-1) \le x \le ih, \\ \frac{(i+1)h - x}{h} & ; & ih < x \le (i+1)h, \\ 0 & ; & \text{elsewhere,} \end{cases}$$

 $(i = 1, 2, 3, \ldots, n-1)$  and

$$\phi_n(x) = \begin{cases} \frac{x - (n-1)h}{h} & ; & (n-i)h < x \le L, \\ 0 & ; & \text{elsewhere.} \end{cases}$$

Here  $h = \frac{L}{n}$  and  $\alpha_i(t)$  are unknown functions to be determined later. Using the Galerkin discretization method with the above spline functions we get the following Cauchy problem with respect to the vector  $\alpha(t)$  having the components  $\alpha_i(t)$ :

$$(2.5) M\alpha'(t) + N\alpha(t) = 0; t > 0,$$

 $\alpha(0)$  is a FEM's interpolation of  $u_0$  [8].

Here

are given  $n \times n$  matrices. Denoting by  $\alpha^j$  the approximation of  $\alpha(t)$  at the time-level  $t_j = \tau_j$  and using the discretization scheme with one parameter (single-step method) to (2.5) we obtain

(2.6) 
$$M\frac{\alpha^{j+1} - \alpha^j}{\tau} + N\left(\gamma \alpha^{j+1} + (1 - \gamma)\alpha^j\right) = 0,$$

where  $\alpha^0=\alpha(0),\ \tau>0$  is a given time-step parameter and  $\gamma\in[0,1]$  is some given parameter, characterizing the time-discretization process. (In case of  $\gamma=0$  it is an explicit scheme,  $\gamma=\frac{1}{2}$  results the Crank-Nicolson scheme and  $\gamma=1$  yields the fully implicit scheme).

The scheme (2.6) can be rewritten in the form

(2.7) 
$$(M + \tau \gamma N)\alpha^{j+1} = (M - \tau (1 - \gamma)N)\alpha^{j}, \quad j = 0, 1, 2, \dots$$

It is clear that for the nonnegativity of all  $\alpha^{j+1}$  vectors the necessary and sufficient condition is the nonnegativity of the matrix

$$(2.8) X = X_1^{-1} X_2,$$

where 
$$X_1 = (M + \tau \gamma N)$$
 and  $X_2 = (M - \tau (1 - \gamma)N)$ .

We shall examine the most trivial sufficient condition for the number

$$q = \frac{\tau}{h^2},$$

resulting the nonnegativity both of the matrices  $X_1^{-1}$  and  $X_2$ . For the matrix  $X_2$  the upper bound yields

$$(2.10) q \le \frac{1}{3(1-\gamma)}.$$

For the linear FEM the matrix  $X_1$  is symmetric, almost uniformly continuant. Thus we can give some sufficient conditions for the nonnegativity of its inverse, using the M-matrix method.

Let us suppose that for some matrix Z the following set of conditions is valid

- (1) Z is a diagonally dominant;
- (2)  $Z_{ii} > 0, i = 1, 2, \ldots, n;$
- (3)  $Z_{ij} \leq 0, i, j = 1, 2, ..., n \quad i \neq j.$

Then Z is an M-matrix and its inverse is nonnegative [1].

**Remark 1.** For the matrix  $X_1$  condition (3) is satisfied only in the case  $q\gamma \geq \frac{1}{6}$ . The conditions 1 and 2 can be checked easily. Hence, we have the following

Theorem 1. If the conditions

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$$(2.11) \frac{1}{6\gamma} \le q \le \frac{1}{3(1-\gamma)}; \quad \gamma \ge \frac{1}{3}$$

are fulfilled, then the solution of the numerical scheme (2.7) conserves the nonnegativity.

It is the same condition which was given in [2] for the first boundary condition in both ends. Moreover, there was proved that the upper bound  $q \leq \frac{1}{3(1-\gamma)}$  is not a necessary condition of the nonnegativity for any n. Our aim is also to get a greater upper bound for q by fixed  $\gamma$ .

### 3. Nonnegativity of the numerical solution of the parabolic problem with third boundary condition

We shall consider the linear parabolic problem with third boundary condition in one dimension having the form

(3.1) 
$$\frac{\partial U}{\partial t} - \frac{\partial^2 U}{\partial x^2} = 0, \quad 0 < x < L,$$

(3.2) 
$$U(x,t) = u_0(x), \quad 0 \le x \le L,$$

(3.3) 
$$\frac{\partial}{\partial x}U(L,t) + cU(L,t) = 0, \quad t \ge 0,$$

$$(3.4) U(0,t) = 0,$$

where c > 0. If we will use the same procedure as in Chapter 2, we get the Cauchy-problem

(3.5) 
$$M\alpha'(t) + N\alpha(t) + B\alpha(t) = 0,$$

 $\alpha(0)$  is a FEM's interpolation of  $u_0$  [8].

Here M and N are defined as earlier and

is a given  $n \times n$  matrix. In this case the nonnegativity of the fully discretized scheme with one parameter can be found by the following way: from (3.5) we get

$$(3.6) M\alpha'(t) + Q\alpha(t) = 0,$$

where Q = N + B. Similarly to (2.10), we get an other upper bound

(3.7) 
$$\tau \le \frac{h^2}{3(1-\gamma)(1+ch)},$$

and at the same time the lower bound does not change

$$\frac{h^2}{6\gamma} \le \tau.$$

So, we have the following

Theorem 2. If the conditions

(3.9) 
$$\frac{h^2}{6\gamma} \le \tau \le \frac{h^2}{3(1-\gamma)(1+ch)}$$

and

$$\frac{3+3ch}{9+3ch} \le \gamma < 1$$

are fulfilled, then the solution of the numerical scheme conserves the nonnegativity for the problem (3.1)-(3.4). If  $\gamma=1$  then the numerical scheme conserves the nonnegativity for the problem (3.1)-(3.4) for any  $\frac{h^2}{6} \leq \tau$ .

A lot of numerical experiments show that the upper bound in (3.9) is not a necessary one. In the next chapter we shall consider our problems in general form.

## 4. Nonnegativity of almost uniformly continuant system of linear algebraic equations

Let us examine our problem in general form

$$(4.1) X_1 y = X_2 b,$$

where

$$(4.2) X_1 = z \begin{bmatrix} x & -1 & 0 & 0 \\ -1 & x & -1 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & 0 & 0 & -1 & x & -1 \\ & & & & 0 & 0 & 0 & -1 & \frac{x}{2} + a \end{bmatrix},$$

$$(4.3) X_2 = \begin{bmatrix} p & s & 0 & 0 \\ s & p & s & 0 \\ \vdots & \vdots & & & \vdots & \vdots & \vdots \\ & & & & 0 & 0 & s & p & s \\ & & & & 0 & 0 & 0 & s & \frac{p}{2} - u \end{bmatrix}$$

are symmetric, almost uniformly continuant matrices of dimension  $n \times n$ ,  $b \in \mathbb{R}^n$  is a given vector,  $y \in \mathbb{R}^n$  is an unknown vector and a and u are given nonnegative numbers.

Without loss of generality we suppose that

$$(4.4) z > 0 and s > 0.$$

If the problem (4.1)-(4.3) arises from the discretezition of some continuous problem having a nonnegative solution, we require the nonnegativity of the discretized problem. (It is, of course, a natural requirement in the practical computations.) It implies the condition of the nonnegativity of the solution y for arbitrary nonnegative vector b. Obviously, this is equivalent with the condition of the nonnegativity of the matrix

$$(4.5) X = X_1^{-1} X_2 \ge 0.$$

If  $X_1$  is an M-matrix and  $X_2$  is nonnegative, then (4.5) is fulfilled. In the case a = u = 0 (that is for the uniformly continuant problem) the condition of the nonnegativity of  $X_2$  can be relaxed for certain negative p's, too ([2], [4], [7]).

We try to do it for the case  $a \neq 0$  and  $u \neq 0$  in the problem (4.1). Let us suppose that  $p \leq 0$ . Making a decomposition of the matrices  $X_1$  and  $X_2$  by the way  $X_1 = X_3 - X_4$  and  $X_2 = X_5 - X_6$  let us introduce the notations:

Now, we can rewrite (4.1) in the form

$$(4.6) (zX_3 - zX_4)y = (X_5 - X_6)b.$$

The inverse G of the matrix  $x_3$  can be given directly [5]

(4.7) 
$$G_{ij} = \begin{cases} \gamma_{i,j} & \text{if } i \leq j, \quad i, j = 1, 2, \dots n, \\ \gamma_{i,j} & \text{if } i > j, \end{cases}$$

where in the case x > 2

(4.8) 
$$\gamma_{i,j} = \frac{\sinh\langle i\vartheta\rangle \sinh\langle n+1-j\rangle\vartheta}{\sinh\langle \vartheta\rangle \sinh\langle n+1)\vartheta}, \quad \vartheta = \operatorname{arch}\left(\frac{x}{2}\right).$$

To get a sufficient condition for the nonnegativity of (4.1) we recall (4.6) and multiply it from its left side by  $\frac{1}{z} X_3^{-1}$ . We obtain

(4.9) 
$$(E - X_3^{-1} X_4) Y = \frac{1}{z} (X_3^{-1} X_5 - X_3^{-1} X_6) b,$$

where E is the identity matrix and

$$X_3^{-1}X_4 = \begin{bmatrix} 0 & 0 & (\frac{x}{2} - a)\gamma_{1n} \\ 0 & 0 & (\frac{x}{2} - a)\gamma_{2n} \\ \vdots & & \vdots \\ 0 & 0 & (\frac{x}{2} - a)\gamma_{nn} \end{bmatrix}$$

is a matrix having nonzero elements only in its last column. Let us notice that  $\gamma_{nn}$  forms a monotonically increasing, convergent sequence with its limit

$$\frac{1}{e^{\vartheta}} = \frac{1}{\frac{x}{2} + \sqrt{\left(\frac{x}{2}\right)^2 - 1}}.$$

Since we need  $(E - X_3^{-1}X_4)$  to be an M-matrix and we know that  $\gamma_{nn} = \max \gamma_{in}$ , we have the condition

$$0 \le \frac{\frac{x}{2} - a}{\frac{x}{2} + \sqrt{\left(\frac{x}{2}\right)^2 - 1}} < 1.$$

This condition yields the restriction

$$(4.10) a \le \frac{x}{2}.$$

So, if (4.10) is fulfilled then the relation  $(E - X_3^{-1}X_4)^{-1} \ge 0$  is valid. Using the results of [2] we can give the matrix  $\frac{1}{2}X_3^{-1}X_5$  in the explicit form

(4.11) 
$$\frac{1}{z}X_3^{-1}X_5 = \frac{1}{z}[(xs+p)G - sE],$$

and formulate the condition of the nonnegativity of this matrix.

It can be easily checked that

$$X_3^{-1}X_6 = \begin{bmatrix} 0 & 0 & (\frac{p}{2} + u) \gamma_{1n} \\ 0 & 0 & (\frac{p}{2} + u) \gamma_{2n} \\ \vdots & \vdots & \vdots \\ 0 & 0 & (\frac{p}{2} + u) \gamma_{nn} \end{bmatrix}.$$

Now, we are able to formulate the sufficient and necessary condition of the non-negativity of the matrix standing on the right side of (4.9). Denoting by  $X_7 = (X_3^{-1}X_5 - X_3^{-1}X_6)$  we need

$$(4.12) X_7 \ge 0.$$

To this end we have to check the condition of the nonnegativity of the last (n-1) column vectors of  $X_7$ , that is we need the condition

$$(4.13) (xs+p)\gamma_{kn} - \left(\frac{p}{2} + u\right)\gamma_{kn} \ge 0, k = 1, 2, \dots, n-1.$$

It yields the restriction

$$(4.14) xs + \frac{p}{2} - u \ge 0,$$

and for k = n it yields the condition for the element  $(X_7)_{nn}$ :

$$(4.15) \gamma_{nn} \ge \frac{s}{xs + \frac{p}{2} - u}.$$

From the other side, we know [2], that for the nonnegativity of the matrix  $X_3^{-1}X_5$ , the necessary and sufficient conditions are

$$(4.16) xs + p > 0,$$

$$(4.17) \gamma_{nn} \ge \frac{s}{xs+p}.$$

So, we have the following

**Theorem 3.** If the conditions (4.10), (4.14), (4.15), (4.16) and (4.17) are fulfilled then (4.1) have a nonnegative solution for arbitrary  $b \ge 0$ .

It is clear that (4.10) guarantees the nonnegativity of the matrix  $(E - X_3^{-1}X_4)^{-1}$ , (4.14), (4.15) are the sufficient conditions of the nonnegativity of

the last column of  $X_7$ . Moreover, the conditions (4.16), (4.17) guarantee the nonnegativity of all other remaining elements of the  $x_7$ .

**Remark 2.** When n = 1, the conditions (4.15) and (4.17) turn into

$$(4.18) \frac{p}{2} - u \ge 0,$$

and

$$(4.19) p \ge 0.$$

The conditions (4.18) and (4.19) show that our sufficient condition is valid for all  $n \in N^+$  only in the case if  $X_2$  is a nonnegative matrix. The relaxed condition p < 0 is working only for n greater than 1. (We mention in practice we have this version, that is, as usual, n is sufficiently large.)

**Remark 3.** Let us consider the case n=2. By using (4.15) and (4.17) we get

$$-\frac{x}{2}p - s + ux \le 0,$$

$$(4.21) -p \le \frac{s}{x}.$$

So, if  $n \ge 2$  and (4.10), (4.14), (4.16), (4.20) and (4.21) are fulfilled then (4.1) conserves the nonnegativity.

Remark 4. The conditions (4.18), (4.19) and (4.20), (4.21) (valid for n = 1 and n = 2, respectively) are sufficient conditions of the nonnegativity. Moreover, for increasing n, always we can find a new sufficient condition for the nonnegativity of (4.1), which is greater than the previous one. It can be done by substituting the value of n into  $\gamma_{nn}$  which appears in (4.15) and (4.17), since

$$\gamma_{nn} = \frac{\sinh(n\vartheta)}{\sinh(n+1)\vartheta}.$$

Hence (4.15) and (4.17) change into the conditions

$$\frac{\sinh(n\vartheta)}{\sinh(n+1)\vartheta} \ge \frac{s}{xs + \frac{p}{2} - u},$$

$$\frac{\sinh(n\vartheta)}{\sinh(n+1)\vartheta} \ge \frac{s}{xs+p}.$$

Knowing the limit value of  $\gamma_{nn}$  we have the following

**Theorem 4.** For the nonnegativity of the matrix  $X_7$  for any space division the necessary conditions are (4.16),

(4.24) 
$$\frac{1}{\frac{x}{2} + \sqrt{\left(\frac{x}{2}\right)^2 - 1}} \ge \frac{s}{xs + \frac{p}{2} - u}$$

and

(4.25) 
$$\frac{1}{\frac{x}{2} + \sqrt{\left(\frac{x}{2}\right)^2 - 1}} \ge \frac{s}{xs + p}.$$

Since we have not explicit form for

$$(4.26) X_8 = (E - X_3^{-1} X_4)^{-1} \cdot X_7,$$

in this case we can talk only about a new sufficient condition of the nonnegativity of (4.1), but we cannot give any necessary conditions as it was done for first boundary condition in [2].

Remark 5. If a = 0, then (4.10) always holds for x > 2.

**Remark 6.** If u = 0 then (4.14) and (4.15) yield

$$(4.27) xs + \frac{p}{2} \ge 0,$$

$$\gamma_{nn} \ge \frac{s}{xs + \frac{p}{2}},$$

respectively. Because the conditions (4.16) and (4.17) are more powerful than (4.27) and (4.28) for the case  $p \leq 0$ , in this case we have to take (4.16) and (4.17) to get a sufficient condition of the nonnegativity of  $X_7$ .

### 5. Sufficient condition of the nonnegativity of second boundary value problems

We want to get a new sufficient condition for the nonnegativity of second boundary value problem. Therefore we recall (2.7) and (4.1). In this case we have for the parameters

(5.1) 
$$z = q\gamma - \frac{1}{6}, \quad x = \frac{\frac{2}{3} + 2\gamma q}{\gamma q - \frac{1}{6}},$$
$$s = \frac{1}{6} + q(1 - \gamma), \quad p = \frac{2}{3} - 2q(1 - \gamma),$$
$$a = 0, \quad u = 0, \quad q\gamma \neq \frac{1}{6}.$$

It is clear that  $x \ge 2$  iff  $\gamma q \ge \frac{1}{6}$ . So we have

Lemma 1. The FEM scheme can be nonnegative for any space division only if

$$(5.2) q \ge \frac{1}{6\gamma}.$$

It is the same lower bound which was given in Theorem 1.

**Remark 7.** The Lemma 1 implies the necessity of the condition  $\gamma > 0$ .

Now we can formulate a new sufficient condition for the nonnegativity of the numerical scheme (2.7) by using Remark 5, Remark 6 and (5.2).

**Theorem 5.** The conditions (4.16), (4.17) by the use of the notation (5.1) guarantee the nonnegativity of the numerical scheme (2.7).

**Remark 8.** For the case n = 2 (4.17) turns to (4.21).

Using (4.21), (5.2) and notations (5.1) we can easily obtain the conditions which preserve the nonnegativity for  $n \ge 2$ .

$$\frac{1}{6\gamma} \le q \le q^*, \quad \gamma \ge \frac{1}{3}.$$

where

(5.4) 
$$q^* = \frac{3(-1+2\gamma) + \sqrt{9-16\gamma(1-\gamma)}}{12\gamma(1-\gamma)}.$$

Remark 9. The condition (5.4) is stronger sufficient condition than the condition (2.11) in case  $n \ge 2$ . Moreover, for increasing n we can always get a new sufficient condition, stronger than (5.4), by using (4.23). So, we have

**Remark 10.** The conditions (4.16), (4.23) and (5.2), by using of the notations (5.1), give a new sufficient condition of the nonnegativity of the scheme (2.7), by fixed n, stronger than (5.4).

### 6. Sufficient condition for the nonnegativity of third boundary value problem

We can find also a new sufficient condition of the nonnegativity of numerical solution for the third boundary value problem. Let us recall (3.6) and after discretization we get a system of linear equations like (4.1), where

$$z = \frac{\tau \gamma}{h^2} - \frac{1}{6}, \quad s = \frac{1}{6} + \frac{\tau}{h^2} (1 - \gamma), \quad x = \frac{\frac{2}{3} + 2\gamma \frac{\tau}{h^2}}{\frac{\tau \gamma}{h^2} + \frac{1}{6}},$$

$$a = \frac{\frac{c}{h} \gamma \tau}{\frac{\tau \gamma}{h^2} - \frac{1}{6}}, \quad u = \frac{c\tau (1 - \gamma)}{h}, \quad \frac{\tau \gamma}{h^2} - \frac{1}{6} \ge 0,$$

$$p = \frac{2}{3} - 2\frac{\tau}{h^2} (1 - \gamma).$$

In Chapter 4 there were given the conditions of the nonnegativity of the equation (4.1). Now, using these results we are able to get new sufficient conditions guaranteeing the nonnegativity of numerical scheme to the problem (3.6).

Remark 11. The nonnegativity of numerical scheme of the problem (3.6) is guaranteed when using the notations (6.1), the conditions (4.10), (4.14), (4.16), (4.20), (4.21) are fulfilled for  $n \ge 2$ .

**Remark 12.** By using Remark 4 we are able to find new stronger sufficient conditions of the nonnegativity by increasing n.

Remark 13. The value c (which appears in equation (3.4)) plays an important effect in changing the upper bound for  $\tau$ . For example, if c is a big value ( $c \ge 1$ ) then  $\tau$ , resulted from (4.20) is smaller than  $\tau$  resulted from (4.21). If (c < 1) then  $\tau$  resulted from (4.21) will be smaller than  $\tau$  resulted from (4.20). Therefore we have to select the minimum value of  $\tau$ , resulted from (4.20) and (4.21) to guarantee the nonnegativity of numerical scheme to the problem (3.6).

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