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NONNEGATIVITY OF THE NUMERICAL SOLUTION OF THREE–DIMENSIONAL HEAT–CONDUCTION EQUATION

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1. Introduction

In this paper we study the nonnegativity of the numerical solution of the three-dimensional heat-conduction problem in a cubic domain. In the one-dimensional case the problem is considered in [3], [5], [7]. In two dimensions this problem is studied in [6]. In this paper - during the discretization process - we use the Descartes product of the basis functions of the one-dimensional linear FEM to the space discretization and the one-step method to the time discretization. We give a sufficient condition of the nonnegativity of the numerical solution.

2. Formulation of the problem

In the domain $\Omega = (0, L) \times (0, L) \times (0, L) \quad (L \in R^+)$ with boundary $\partial\Omega$, we consider linear parabolic problem having the form:

$$\frac{\partial u}{\partial t} - \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = 0, \qquad (x, y, z) \in \Omega, \quad t > 0, \tag{2.1}$$

$$u(x, y, z, 0) = u_0(x, y, z), \qquad (x, y, z) \in \overline{\Omega}, \tag{2.2}$$

$$u(x, y, z, t) = 0, \qquad (x, y, z) \in \partial\Omega, \quad t > 0. \tag{2.3}$$

Under some natural conditions (i.e. the initial function u_0 is sufficiently smooth and nonnegative) the solution of the problem (2.1)-(2.3) is nonnegative on the whole domain $\Omega \times R_0^+$ [4], [9]. This property plays an important role in applications, (2.1)-(2.3) describes the process of heat conduction. Our goal is to formulate the conditions of conservation of this property in the case of the Galerkin type numerical solutions. First, we apply the Descartes product of the basis functions of the one-dimensional linear FEM to the space-discretization. Secondly, we use the one-step method for the time discretization. We give some sufficient conditions for the conservation of the nonnegativity of the fully discretized scheme.

The weak form of the problem (2.1)-(2.3) is

$$\int_0^L\int_0^L\int_0^L \left(\frac{\partial u}{\partial t}v + \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} + \frac{\partial u}{\partial z}\frac{\partial v}{\partial z}\right) dxdydz = 0; \quad \forall v \in H_0^1(\Omega). \tag{2.4}$$

Let us divide the domain Ω into the subdomains

$$\Omega_{ijk} = [x_{i-1}, x_i] \times [y_{j-1}, y_j] \times [z_{k-1}, z_k] \quad \text{where} \quad x_i = ih,\ y_j = jh,\ z_k = kh,$$

$i, j, k = 1, 2, \ldots, n$. Denote by $\Phi_i(x)$ the linear spline function at points x_i. We define the set of basis functions

$$\Phi_{ijk}(x, y, z) = \Phi_i(x)\Phi_j(y)\Phi_k(z), \quad (x, y, z) \in \Omega_{ijk} \tag{2.5}$$

for all $i, j, k = 1, 2, \ldots, n-1$ and seek the numerical solution in the form

$$U_h(x, y, z, t) = \sum_{i=1}^{n-1}\sum_{j=1}^{n-1}\sum_{k=1}^{n-1} \alpha_{ijk}(t)\Phi_{ijk}(x, y, z). \tag{2.6}$$

Here n is the number of subdomains in each direction, $h = \frac{L}{n}$, $\alpha_{ijk}(t)$ are unknown functions to be determined later.

Substituting (2.6) into (2.4) we get a Cauchy problem for the vector $\alpha(t) = [\alpha_{ijk}(t)]_{ijk=1}^{n-1}$ of the form

$$M\alpha'(t) + Q\alpha(t) = 0 \qquad t > 0, \tag{2.7}$$

where $\alpha(0)$ is a given vector being an approximation of the initial function u_0.

Here we have used the following notations:

$$\overline{H} = \text{tridiag}[1, 4, 1] \in R^{(n-1)\times(n-1)}; \quad M_1 = \frac{2}{27}\overline{H},\ M_2 = \frac{1}{54}\overline{H}$$

and

$$M_3 = \frac{1}{216}\overline{H};$$

$\hat{M}_4,\ \hat{M}_5$ are hypermatrices having the form

$$\hat{M}_4 = \text{tridiag}[M_3, M_2, M_3], \qquad \hat{M}_5 = \text{tridiag}[M_2, M_1, M_2]$$

and

$$M = \text{tridiag } h^3[\hat{M}_4, \hat{M}_5, \hat{M}_4] \in R^{(n-1)^3\times(n-1)^3}.$$

Similarly,

$$N_1 = \frac{2}{9}\overline{H},\ N_2 = \frac{1}{18}\overline{H},\ N_3 = -\frac{1}{9}\overline{H},\ N_4 = -\frac{1}{36}\overline{H};$$

$\hat{N}_4,\ \hat{N}_5$ are hypermatrices having the form

$$\hat{N}_4 = \text{tridiag}[N_4, N_3, N_4], \quad \hat{N}_5 = \text{tridiag}[N_2, N_1, N_2]$$

and

$$N = \text{tridiag } h[\hat{N}_4, h\hat{N}_5, \hat{N}_4] \in R^{(n-1)^3\times(n-1)^3}.$$

Analogically,

$$C_1 = \frac{2}{9}\overline{H}, C_2 = -\frac{1}{9}\overline{H},\ C_3 = \frac{1}{18}\overline{H},\ C_4 = -\frac{1}{36}\overline{H};$$

$\hat{C}_4,\ \hat{C}_5$ are hypermatrices having the form

$$\hat{C}_4 = \text{tridiag}[C_4, C_3, C_4], \quad \hat{C}_5 = \text{tridiag}[C_2, C_1, C_2]$$

and

$$C = \text{tridiag } h[\hat{C}_4, \hat{C}_5, \hat{C}_4] \in R^{(n-1)^3\times(n-1)^3}.$$

In the same way

$$\overline{F} = \text{tridiag}[-1, 2, -1] \in R^{(n-1)\times(n-1)}; \quad B_1 = \frac{4}{9}\overline{F},\ B_2 = \frac{1}{9}\overline{F},\ B_3 = \frac{1}{36}\overline{F};$$

B_4, B_5 are hypermatrices having the form

$$\hat{B}_4 = \text{tridiag}[B_3, B_2, B_3], \quad \hat{B}_5 = \text{tridiag}[B_2, B_1, B_2]$$

and

$$B = \text{tridiag } h[\hat{B}_4, \hat{B}_5, \hat{B}_4] \in R^{(n-1)^3\times(n-1)^3}.$$

$Q = N + C + B$, we get $Q_1, Q_2, Q_3 \in R^{(n-1)\times(n-1)}$, where

$$Q_1 = \frac{8}{3}I \ (I \text{ is identity matrix}), \quad Q_2 = \text{tridiag}\left[-\frac{1}{6}, 0, -\frac{1}{6}\right],$$

$$Q_3 = \text{tridiag}\left[-\frac{1}{12}, -\frac{1}{6}, -\frac{1}{12}\right];$$

$\hat{Q}_4, \hat{Q}_5$ are hypermatrices where

$$\hat{Q}_4 = \text{tridiag}[Q_3, Q_2, Q_3], \quad \hat{Q}_5 = \text{tridiag}[Q_2, Q_1, Q_2],$$

then it is easy to see $Q = \text{tridiag}\ h[\hat{Q}_4, \hat{Q}_5, \hat{Q}_4] \in R^{(n-1)^3\times(n-1)^3}$.

Using the one-step method to the discretization of (2.7) we get the system of linear algebraic equations

$$X_1\alpha^{j+1} = X_2\alpha^j, \qquad j = 0, 1, 2, \ldots, \tag{2.8}$$

where $X_1 = M + \tau\gamma Q,\ X_2 = M - \tau(1-\gamma)Q,\ \alpha^j$ is the approximation of $\alpha(t)$ time-level $t_j = \tau j,\ \tau > 0$ is the time-step parameter and $\gamma \in [0, 1]$ is a given parameter. We remark that α^0 is an appropriate approximation of the initial function at the points of the mesh, namely, we can take $(\alpha^0)_{i,j,k} = u_0(x_i, y_j, z_k)$. So, if $u_0 \geq 0$ then $\alpha^0 \geq 0$.

3. Nonnegativity of full discretization

We need the nonnegativity of the matrix

$$X = X_1^{-1}X_2.$$

The most trivial condition of the nonnegativity of X is the conditions $X_1^{-1} \geq 0$ and $X_2 \geq 0$. We give some condition for the number $q = \dfrac{\tau}{h^2}$ which guarantees these conditions.

For the matrix X_2 we can do it directly and it results the upper bound

$$q \leq \frac{1}{9(1-\gamma)}. \tag{3.1}$$

In the case of the matrix X_1 we are not able to get a sufficient condition for the nonnegativity of the matrix X_1^{-1} by the M-matrix method [1]. (Like it was done for one and two dimensional cases [3], [5], [6], [7].) It follows from the fact that X_1 always contains some positive elements in its off-diagonal. But by using Theorem 3 in [8] we can give some other sufficient condition for the nonnegativity.

For this aim we decompose X_1 into the following matrices: the diagonal part $(X_1)_d$, the positive off-diagonal part X_1^+ and two negative off-diagonal parts X_1^z and X_1^s, where X_1^z is an upper triangle negative element of X_1 and X_1^s is a lower triangle negative element of X_1. One can check that in the case

$$\frac{2}{27} \le \frac{\left(\frac{1}{54} - \frac{1}{6}q\gamma\right)\left(\frac{1}{216} - \frac{1}{12}q\gamma\right)}{\frac{8}{27} + \frac{8}{3}q\gamma}, \tag{3.2}$$

all conditions of the above theorem are satisfied. The inequality (3.2) results the bound

$$\frac{259 + 13\sqrt{409}}{36\gamma} \le q. \tag{3.3}$$

So, we have

Theorem 1. *If the conditions*

$$\frac{259 + 13\sqrt{409}}{36\gamma} \le q \le \frac{1}{9(1-\gamma)}; \qquad 0.992395 \le \gamma < 1, \tag{3.4}$$

$$\frac{259 + 13\sqrt{409}}{36} \le q \qquad \gamma = 1$$

are fulfilled then the solution of the numerical scheme (2.8) remains nonnegative for any initial nonnegative vector α^0.

Obviously, the upper bound in (3.4) is a sufficient condition for the nonnegativity of numerical scheme (2.8). To get a greater upper bound let us apply the process given in [10].

Denoting by

$$T = \begin{bmatrix} I & 0 \\ -X_2 & X_1 \end{bmatrix},$$

where I is the identity matrix of dimension $(n-1)^3 \times (n-1)^3$, the problem (2.8) can be rewritten in the form

$$T \begin{bmatrix} \alpha^j \\ \alpha^{j+1} \end{bmatrix} = \begin{bmatrix} \alpha^j \\ 0 \end{bmatrix}. \tag{3.5}$$

So, if under some conditions (3.5) conserves the nonnegativity then under the same conditions (2.8) also does it. Therefore we examine the condition T to be an inverse nonnegative (monotone) matrix. For this aim, we are going to apply Theorem 3 in [8]. We partition T into the diagonal part T_d, the positive off-diagonal part T^+ and two negative off-diagonal parts T^Z and T^S. Denoting by

$$T_d = \begin{bmatrix} I & 0 \\ 0 & t_d I \end{bmatrix}, \; T^+ = \begin{bmatrix} 0 & 0 \\ -X_2^- & 0 \end{bmatrix}, \; T^Z = \begin{bmatrix} 0 & 0 \\ 0 & X_1^- \end{bmatrix}, \; T^S = \begin{bmatrix} 0 & 0 \\ -X_2^+ & 0 \end{bmatrix},$$

we obtain, that in case

$$p \leq \frac{3s_1 t_1^- + s_2 t_2^-}{t_d}, \tag{3.6}$$

all conditions of above theorem hold. Here we have used the notations

$$p = -\left[\frac{8}{27} - \frac{8}{3}q(1-\gamma)\right], \; s_1 = -\left[\frac{1}{54} + \frac{1}{6}q(1-\gamma)\right],$$

$$s_2 = -\left[\frac{1}{216} + \frac{1}{12}q(1-\gamma)\right], \; t_d = \frac{8}{27} + \frac{8}{3}q\gamma, \; t_1^- = \frac{1}{54} - \frac{1}{6}q\gamma,$$

$$t_2^- = \frac{1}{216} - \frac{1}{12}q\gamma.$$

So, (3.6) results the upper bound

$$q \leq \frac{691(2\gamma - 1) + \sqrt{91472\gamma^2 - 91472\gamma + 477481}}{12132\gamma(1-\gamma)}. \tag{3.7}$$

Summarizing our conditions, we have the following

Theorem 2. *If q satisfies the conditions*

$$\frac{259 + 13\sqrt{409}}{36\gamma} \leq q \leq \frac{691(2\gamma - 1) + \sqrt{91472\gamma^2 - 91472\gamma + 477481}}{12132\gamma(1-\gamma)}, \tag{3.8}$$

and

$$0.9923 \leq \gamma < 1,$$

then in case $n \geq 4$ the numerical scheme (2.8) conserves the nonnegativity for any nonnegative vector α^0.

Remark 1. Let us substitute $\gamma = 0.995$ into (3.4) and (3.8). It leads to the bounds

$$14.5703 \le q \le 22.2222,$$

and

$$14.5703 \le q \le 22.7773,$$

respectively.

Analogically, if we substitute $\gamma = 0.9999$ into (3.4), (3.8), we obtain

$$14.4989 \le q \le 1111.11,$$

$$14.4989 \le q \le 1139.13.$$

Under the condition (3.8) T is monotone and since $T \begin{bmatrix} e \\ e \end{bmatrix} \ge 0$ (where e$=[1,1,1,\ldots]^T \in R^{(n-1)^3}$) so the maximum principle also holds [2]. From this fact we can prove directly the monotone convergence of the numerical scheme (2.8) in maximum norm. Since the numerical scheme satisfies the maximum principle and at each time level the solution is nonnegative, we have

$$\max_{1 \le i \le (n-1)^3} \alpha_i^{j+1} \le \max_{1 \le i \le (n-1)^3} \alpha_i^j .$$

Using the notation

$$\left\| \alpha^j \right\|_c = \max_{1 \le i \le (n-1)^3} \left| \alpha_i^j \right| ,$$

we get immediately

$$\left\| \alpha^{j+1} \right\|_c \le \left\| \alpha^j \right\|_c , \tag{3.9}$$

which means the monotone convergence of the numerical scheme (2.8) in maximum norm.

Remark 2. Let us consider instead of (2.1) the equation

$$\frac{\partial u}{\partial t} - k \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = 0, \qquad (x,y,z) \in \Omega, \quad t > 0,$$

where $k > 0$ is a given constant. Repeating the same calculation instead of (3.4) we get the bound

$$\frac{259 + 13\sqrt{409}}{36k\gamma} \le q \le \frac{1}{9k(1-\gamma)}; \qquad 0.992395 \le \gamma < 1$$

and instead of (3.8) we get

$$\frac{259+13\sqrt{409}}{36k\gamma} \leq q \leq \frac{691(2\gamma-1)+\sqrt{91472\gamma^2-91472\gamma+477481}}{12132k\gamma(1-\gamma)},$$

$$0.9923 \leq \gamma < 1.$$

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