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Nonstandard Finite Difference Schemes for Reaction-Diffusion Equations

T. Zhanlav * , B. Batgerel †

* Department of Applied Mathematics School of Mathematics and Computer Science National University of Mongolia, Mongolia

† Department of Natural Science School of Technology in Darkhan Mongolian University of Science and Technology, Mongolia

A nonstandard, implicit finite difference scheme for reaction-diffusion equation was constructed. This scheme is an extension of the method of Mickens. Conditions of positivity and boundedness are established.

Key words and phrases: reaction-diffusion equation, nonstandard finite difference scheme, positivity, boundedness.

1. Introduction

As is known, [1,2], a large class of important phenomena in the natural and engineering sciences can be represented by a system of nonlinear reaction-diffusion PDEs in one-space dimension:

$$\frac{\partial u_i}{\partial t} = D_i \frac{\partial^2 u_i}{\partial x^2} + f_i(u_1, u_2, \dots, u_n) u_i, \quad i = 1, 2, \dots, n,$$
(1)

where D_i are nonnegative diffusion coefficients, and the f_i are rational functions of (u_1, u_2, \ldots, u_n) . We restrict the discussion to systems modeled by (1) for which the $u_i(x,t)$ represent density variables. Consequently,

$$u_i(x,0) \geqslant 0 \quad \Rightarrow \quad u_i(x,t) \geqslant 0,$$

which is a positivity condition on the dependent variables.

We will consider the system of equations (1) along with the initial condition

$$u_i(x,0) = \varphi_i(x) \geqslant 0, \quad x \in (0,l), \tag{2}$$

and either Dirichlet boundary conditions

$$u_i(0,t) = \omega_i(t), \quad u_i(l,t) = \vartheta_i(t),$$
 (3)

or Neumann boundary conditions

$$\frac{\partial u_i}{\partial x}(0,t) = -\omega_i(t), \quad \frac{\partial u_i}{\partial x}(l,t) = \vartheta_i(t), \tag{4}$$

where $\omega_i(t) \ge 0$, $\vartheta_i(t) \ge 0$ are given functions.

We will use the following notations:

$$t \to t_k = k\tau, \quad k = 0, 1, \dots, \quad x \to x_m = mh, \quad m = 0, 1, \dots, N,$$

where τ and h are, respectively, the time and space step-sizes; and the discrete approximations to the dependent variables are

$$u_i(x_m, t_k) \to [y_i]_m^k, \quad i = 1, 2, \dots, n.$$

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2. The Nonstandard Finite Difference Schemes

In this article we consider a nonstandard finite difference schemes of the form

$$\frac{[y_i]_m^{k+1} - [y_i]_m^k}{\tau} = D_i \left((1 - \sigma)[y_i]_{\overline{x}x,m}^k + \sigma[y_i]_{\overline{x}x,m}^{k+1} \right) + dp_i(y)[y_i]_m^k - ((d-1)p_i(y) + q_i(y))[y_i]_m^{k+1}, \quad (5)$$

where $\sigma \in [0,1]$ and $d \ge 1$ are parameters and $p_i(y)$ and $q_i(y)$ are, respectively, the collection of functions obtained from the positive and negative coefficient terms in f_i . Note that $p_i(y)$ and $q_i(y)$ are evaluated at t_k and x_m i.e., in detail

$$p_i(y) = p_i ([y_1]_m^k, [y_2]_m^k, \dots, [y_n]_m^k),$$

$$q_i(y) = q_i ([y_1]_m^k, [y_2]_m^k, \dots, [y_n]_m^k).$$

The functions $p_i(y)$ and $q_i(y)$ also have the important property

$$p_i(y) \ge 0$$
, $q_i(y) \ge 0$ if $[y_i]_m^k \ge 0$, $i = 1, 2, ..., n$.

Note that the schemes (5) are implicit in general and we rewrite them as follows:

$$-a_m[y_i]_{m-1}^{k+1} + c_m[y_i]_m^{k+1} - b_m[y_i]_{m+1}^{k+1} = F([y_i]_m^k),$$
(6)

where

$$a_{m} = b_{m} = \sigma \gamma D_{i}, \quad \gamma = \frac{\tau}{h^{2}},$$

$$c_{m} = 1 + 2\sigma \gamma D_{i} + \tau \left((d-1)p_{i}(y) + q_{i}(y) \right),$$

$$F\left([y_{i}]_{m}^{k} \right) = (1 - \sigma)\gamma D_{i} \left([y_{i}]_{m-1}^{k} + [y_{i}]_{m+1}^{k} \right) + (1 + d\tau p_{i}(y) - 2(1 - \sigma)\gamma D_{i}) \left[y_{i} \right]_{m}^{k}.$$
(7)

The discrete initial conditions are

$$[y_i]_m^0 = \varphi_i(x_m), \quad m = 0, 1, \dots, N.$$
 (8)

The discrete boundary conditions corresponding to (3), (4) are

$$[y_i]_0^k = \omega_i(t_k), \quad [y_i]_N^k = \vartheta_i(t_k), \quad k = 0, 1, \dots,$$
 (9)

and

$$\frac{[y_i]_1^k - [y_i]_{-1}^k}{2h} = -\omega_i(t_k), \quad \frac{[y_i]_{N+1}^k - [y_i]_{N-1}^k}{2h} = \vartheta_i(t_k), \quad (10)$$

respectively. The equations (6) together with (8), (9) or (8), (10) must be form a closed system.

We first consider the discrete Dirichlet boundary condition (9). Since $[y_i]_0^{k+1}$ and $[y_i]_N^{k+1}$ are known via the condition (9), we can transfer these quantities from equation (6) for m=1 and m=N-1 to the right hand side respectively. As a result we obtain

$$\begin{cases}
c_1[y_i]_1^{k+1} - b_1[y_i]_2^{k+1} = F([y_i]_1^k), \\
-a_m[y_i]_{m-1}^{k+1} + c_m[y_i]_m^{k+1} - b_m[y_i]_{m+1}^{k+1} = F([y_i]_m^k), \quad m = 2, \dots, N-2, \\
-a_{N-1}[y_i]_{N-2}^{k+1} + c_{N-1}[y_i]_{N-1}^{k+1} = F([y_i]_{N-1}^k),
\end{cases}$$
(11)

where

$$F([y_i]_1^k) = a_1 \omega_i (t_{k+1}) + (1 - \sigma) \gamma D_i (\omega_i (t_k) + [y_i]_2^k) +$$

+
$$(1 + d\tau p_i(y) - 2(1 - \sigma)\gamma D_i) [y_i]_1^k$$
, (12)

$$F([y_i]_{N-1}^k) = b_{N-1}\vartheta(t_{k+1}) + (1-\sigma)\gamma D_i(\vartheta(t_k) + [y_i]_{N-2}^k) + (1 + d\tau p_i(y) - 2(1-\sigma)\gamma D_i)[y_i]_{N-1}^k.$$

Now we proceed to the discrete Neumann boundary condition (10). As in [3,4] the discrete boundary conditions (10) are incorporated by introducing the auxiliary points $x_{-1} = x_0 - h$ and $x_{N+1} = x_N + h$. By using the difference equation (6) at m = 0 and first relation in (10), we can eliminate the unknown $[y_i]_{N+1}^k$. And, of course, the unknown $[y_i]_{N+1}^k$ can be eliminated in a similar way. As a result, we obtain

$$\begin{cases}
c_0[y_i]_0^{k+1} - 2b_0[y_i]_1^{k+1} = F([y_i]_0^k), \\
-a_m[y_i]_{m-1}^{k+1} + c_m[y_i]_m^{k+1} - b_m[y_i]_{m+1}^{k+1} = F([y_i]_m^k), \quad m = 1, \dots, N-1, \\
-2a_{N-1}[y_i]_{N-1}^{k+1} + c_N[y_i]_N^{k+1} = F([y_i]_N^k),
\end{cases}$$
(13)

where

$$F([y_i]_0^k) = 2h\gamma D_i (\sigma\omega_i(t_{k+1}) + (1 - \sigma)\omega_i(t_k)) + 2(1 - \sigma)\gamma D_i [y_i]_1^k + (1 + d\tau p_i(y) - 2(1 - \sigma)\gamma D_i) [y_i]_0^k, \quad (14)$$

$$F([y_i]_N^k) = 2h\gamma D_i(\sigma \vartheta_i(t_{k+1}) + (1 - \sigma)\vartheta_i(t_k)) + 2(1 - \sigma)\gamma D_i[y_i]_{N-1}^k + (1 + d\tau p_i(y) - 2(1 - \sigma)\gamma D_i)[y_i]_N^k.$$

We are ready to show that

Theorem 1. The positivity condition holds under condition

$$(1 - \sigma)\gamma \leqslant \frac{1 + d\tau p_i}{2D_i}, \quad i = 1, \dots, n.$$

$$(15)$$

Proof. The systems of equations (11) and (13) can be rewritten as a matrix from

$$A [y_i]^{k+1} = F ([y_i]^k).$$

It is easy to see that the tri-diagonal matrix A is a strictly diagonally dominant and monotone type. Moreover, from (7), (12) and (14), it follows that

$$F\left(\left[y_{i}\right]\right)^{k}\geqslant0,$$

under the assumptions $[y_i]_m^k \ge 0$ and (15). The Theorem 1 has proved.

Now we consider a boundedness property of the solution to (1), (2) and (3)–(4).

Theorem 2. Assume that

- (i) $0 \le [y_i]_m^k \le M, \quad m = 0, 1, \dots, N,$
- (ii) the condition (1.21) holds,

(iii)
$$(1 + d\tau p_i(y) - 2(1 - \sigma)\gamma D_i) \left(M - [y_i]_m^k \right) \geqslant M\tau \left(p_i(y) - q_i(y) \right),$$

 $m = 1, 2, \dots, N - 1.$

Then

$$0 \leqslant [y_i]_m^{k+1} \leqslant M$$
 for all $m = 0, 1, \dots, N$.

Proof. Theorem 1 is valid under assumptions (i) and (ii), i.e., $[y_i]_m^{k+1} \ge 0$ for all m = 0, 1, ..., N. Moreover, we have [5]

$$\max_{m} [y_i]_m^{k+1} \leqslant \frac{F([y_i]_m^k)}{r_m},$$

where

$$r_m = c_m - a_m - b_m.$$

It is easy to seen that the condition (iii) is sufficient for

$$\frac{F\left([y_i]_m^k\right)}{r_m} \leqslant M.$$

It means that $[y_i]_m^{k+1} \leq M$ for all m = 0, 1, ..., N, which completes the proof of Theorem 2.

Remark. The positivity condition (15) is valid for any time and space step sizes τ , h for implicit scheme (5) with $\sigma = 1$.

3. Applications

We consider some particular cases of problem (1), (2) and (3). *The Nagumo equation.* Now, we consider the reaction-diffusion equation

$$u_t = Du_{xx} + (\alpha - \beta u^2) u, \quad 0 \leqslant x \leqslant L, \quad t > 0$$

with D > 0, $\alpha > 0$, $\beta > 0$ and

$$0 \leqslant u(x,t) \leqslant \sqrt{\frac{\alpha}{\beta}}$$
.

The difference scheme is

$$\frac{y_m^{k+1} - y_m^k}{\tau} = D\left((1 - \sigma) y_{\overline{x}x,m}^k + \sigma y_{\overline{x}x,m}^{k+1} \right) + d\alpha y_m^k - \left((d - 1)\alpha + \beta \left(y_m^k \right)^2 \right) y_m^{k+1}.$$

The positivity and boundedness of the solutions is satisfied if the condition

$$(1-\sigma)\gamma \leqslant \frac{1+(d-2)\tau\alpha}{2D}$$

holds.

Finally, we consider a set of PDEs:

$$\frac{\partial u_1}{\partial t} = D_1 \frac{\partial^2 u_1}{\partial x^2} + [f(u_1) - u_2] u_1,$$

$$\frac{\partial u_2}{\partial t} = D_2 \frac{\partial^2 u_2}{\partial x^2} + [u_1 - g(u_2)] u_2,$$
(16)

where

$$f(u_1) = a(a_1 + b_1u_1 - u_1^2), \quad g(u_2) = a_2 + b_2u_2,$$

and a, a_1 , a_2 , b_1 , b_2 are nonnegative parameters. This system is a model for the description of the patchy distributions of microscopic aquatic organisms and was constructed by Mimura and Mirray.

The finite difference scheme for this set of equations is

$$\frac{y_m^{k+1} - y_m^k}{\tau} = D_1 \left[(1 - \sigma) y_{\overline{x}x,m}^k + \sigma y_{\overline{x}x,m}^{k+1} \right] + da \left(a_1 + b_1 y_m^k \right) y_m^k - \left[(d - 1) a \left(a_1 + b_1 y_m^k \right) + a \left(y_m^k \right)^2 + w_m^k \right] y_m^{k+1},$$

$$\frac{w_m^{k+1} - w_m^k}{\tau} = D_2 \left[(1 - \sigma) w_{\overline{x}x,m}^k + \sigma w_{\overline{x}x,m}^{k+1} \right] + dy_m^k w_m^k - \left[(d - 1) y_m^k + a_2 + b_2 w_m^k \right] w_m^{k+1}.$$

The positivity condition becomes

$$\gamma(1-\sigma) \leqslant \frac{1}{2D}, \quad D = \min(D_1, D_2).$$

One can check that the sufficient boundedness requirement (iii) with M=1 is fulfilled

$$a > 0, \quad a_2 \ge 1, \quad b_2 \ge 0, \quad a_1 + b_1 \le 1, \quad d = \frac{a_1 + b_1}{b_1} \ge 1.$$
 (17)

From (17), we can see that the parameter $d \ge 1$ plays as a control parameter. So, by choosing the value of d in suitable way, one can satisfy boundedness requirement for solution of (17).

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Нестандартные конечно-разностные схемы для уравнений реакции-диффузии

Т. Жанлав*, Б. Батгэрэл†

* Кафедра прикладной математики Математический факультет Монгольский государственный университет, Монголия

† Кафедра естественных наук Дарханский технологическии институт Монгольский государственный университет науки и технологий, Монголия

Построена нестандартная, неявная конечно-разностная схема для уравнения реакциидиффузии. Эта схема является обобщением метода Микенса. Установлены условия положительности и ограниченности решения.

Ключевые слова: уравнения реакции-диффузии, нестандартная конечно-разностная схема, положительность и органиченность.