Reduction of a boundary value problem for a system of diffusion-reaction equations to problem for a finite interval

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Abstract. The boundary value problem on a semi-infinite interval for a system of ordinary differential equations of the diffusion-reaction type is considered. To apply a difference scheme for the numerical solution of such a problem, it is necessary to reduce it to a problem for a finite interval. For this perpose we offer to use well-known method of construction of the stable variety of solutions that satisfy the limit condition at infinity. The estimates of the error arising when the problem is reduced to a finite interval are obtained.

1. Introduction

Various convective-diffusion processes are modeled on the basis of differential equations and of systems with a small parameter before higher derivatives. Solutions of such problems have large gradients in the boundary layer. This must be considered when building computational algorithms [1]. In mathematical modeling of a number of physical processes, for example, the transfer of impurities or chemical reactions, the limiting boundary conditions are set at infinity. To solve numerically such problem, it is necessary to reduce this problem to a finite domain. In this paper, we consider the problem of reducing the problem to a finite interval in the case of a linear system of ordinary differential equations with a limit boundary condition at infinity.

We consider a boundary value problem for a linear system of differential equations of diffusion-reaction type on a semi-infinite interval. We use the method of reducing a problem to a finite interval on the basis of extracting a variety of solutions satisfying a given condition at infinity. The method of transferring conditions from a singular point was proposed by A.A. Abramov [2] and developed in a number of works by A.A. Abramov, N.B. Konyukhova and their co-authors in [3], [4] and in other works. It is shown how the developed approach can be applied in the case of a parabolic equation on the half-line.

Now we introduce the notation. The Euclidean norm for vectors and the spectral norm for matrices are used. It is assumed that a matrix is nonnegative if its eigenvalues do not lie in the left half-plane. By C and C_i, we mean positive constants that independent of the parameter ε and grid steps.

2. A boundary value problem for a system of equations on a semi-infinite interval

Consider the boundary problem for the system of equations reaction-diffusion type on a semi-infinite interval

$$\varepsilon^2 \mathbf{U}''(x) - P(x)\mathbf{U}(x) = \mathbf{F}(x), \tag{1}$$

$$\mathbf{U}(0) = \mathbf{A}, \quad \lim_{x \to \infty} \mathbf{U}(x) = \mathbf{0}. \tag{2}$$

We assume that the vector function $\mathbf{F}(x)$ of order n and the matrix $P(x)$ of order $n \times n$ are sufficiently smooth in the variable x. Let the matrix $P(x)$ be positive definite,

$$\varepsilon \in (0, 1], \ P(x) \geq \alpha I, \alpha > 0, \ \lim_{x \to \infty} P(x) = P_\infty, \ \lim_{x \to \infty} \mathbf{F}(x) = \mathbf{0}.$$

In part, the problem (1)-(2) was investigated in [5], where the following stability estimate is proved

$$\max_x ||\mathbf{U}(x)|| \leq \sqrt{\frac{1}{\alpha^2} \max_x ||\mathbf{F}(x)||^2 + ||\mathbf{A}||^2}, \ x \geq 0, ||\mathbf{U}|| = \Big\{ \sum_{k=1}^n U_k^2 \Big\}^{1/2}. \tag{3}$$

We investigate the method of reduction of the problem (1)-(2) to finite interval based on the extraction of the variety of solutions satisfying the limit condition at infinity [4].

So, we define the desired variety as the set of solutions of a system of equations of the first order:

$$\varepsilon \mathbf{W}'(x) + G(x)\mathbf{W}(x) = \beta(x), \tag{4}$$

where the matrix $G(x)$ is the solution of the singular Cauchy problem for the matrix Riccati equation:

$$\varepsilon G'(x) - G^2(x) + P(x) = 0, \ \lim_{x \to \infty} G(x) = \sqrt{P_\infty}, \tag{5}$$

and the vector function $\beta(x)$ is a solution of singular Cauchy problem

$$\varepsilon \beta'(x) - G(x)\beta(x) = \mathbf{F}(x), \ \lim_{x \to \infty} \beta(x) = 0. \tag{6}$$

The equations (5), (6) are defined so that the solution of equation (4) is a solution to the original equation (1).

Let us dwell on the properties of the solution of the problem (5). In accordance with [5] $G(x) \geq \sqrt{\alpha}I$ if $x \geq 0$.

In accordance with [6], the following lemma is true.

Lemma 1 *Let $U(x)$ be a symmetric matrix with $x \leq r$,*

$$LU = \varepsilon U'(x) - Q(x)U(x) - U(x)S(x).$$

Then from the conditions:

$$U(r) \geq 0, \ LU(x) \leq 0, \ x < r$$

it follows that $U(x) \geq 0$ for all $x < r$.

Here, under the inequality $U(x) \geq 0$ it is assumed that all the eigenvalues of this matrix are not negative.

Lemma 2 *Let $U(x)$ be a solution of matrix problem*

$$\varepsilon U'(x) - Q(x)U(x) - U(x)S(x) = F(x), \quad U(r) = U_0,$$

$U(x)$ is symmetric matrix, $Q(x) \geq \beta I$, $S(x) \geq \omega I$, $\beta > 0, \omega > 0$. Then for all $x \leq r$

$$||U(x)|| \leq ||U_0|| + \frac{1}{\beta + \omega} \max_x ||F(x)||.$$

The proof of this lemma is based on the use of the maximum principle, which takes a place in accordance with lemma 1.

Now we investigate the stability of the solution of the problem (5) to perturbation of the matrix $P(x)$.

Lemma 3 *Let $P(x)$ and $\tilde{P}(x)$ are symmetric matrices, $\tilde{G}(x)$ is the solution of the problem (5) in the case of the matrix $\tilde{P}(x)$, where $\tilde{P}(x) \geq \tilde{\alpha}$. Then for all $x \geq 0$*

$$||G(x) - \tilde{G}(x)|| \leq ||\sqrt{P_\infty} - \sqrt{\tilde{P}_\infty}|| + \frac{1}{\sqrt{\alpha} + \sqrt{\tilde{\alpha}}} \max_x ||P(x) - \tilde{P}(x)||.$$

Proof. Putting $U(x) = G(x) - \tilde{G}(x)$, we get

$$LU(x) = \varepsilon U'(x) - G(x)U(x) - U(x)\tilde{G}(x) = \tilde{P}(x) - P(x),$$

$$\lim_{x \to \infty} U(x) = \sqrt{P_\infty} - \sqrt{\tilde{P}_\infty}.$$

The matrix $U(x)$, as the difference of two symmetric matrices, is symmetric. Lemma 2 implies the assertion of the lemma.

Thus, in the case of a symmetric matrix $P(x)$, the problem (5) has the only solution that is stable to perturbation of the matrix $P(x)$, which leaves the matrix symmetric.

Using $\tilde{G}(x) = 0$, $\tilde{P}(x) = 0$, from lemma 3 we get

$$||G(x)|| \leq ||\sqrt{P_\infty}|| + \frac{1}{\sqrt{\alpha}} \max_x ||P(x)||.$$

Lemma 4 *For the solution of the problem (6) the following estimate is true*

$$\max_{x \geq L} ||\beta(x)|| \leq \frac{2}{\sqrt{\alpha}} \max_{x \geq L} ||\mathbf{F}(x)||$$

for any $L \geq 0$.

Proof. Multiply the equation (6) scalarly by $\beta(x)$:

$$\varepsilon(\beta'(x), \beta(x)) - (G(x)\beta(x), \beta(x)) = (\mathbf{F}(x), \beta(x)).$$

Let us $w(x) = (\beta(x), \beta(x))$. Then

$$\frac{\varepsilon}{2}w' - \sqrt{\alpha}w \geq (\mathbf{F}, \beta).$$

We account the inequality $2|(\mathbf{F}, \beta)| \leq \sigma||\beta||^2 + \sigma^{-1}||\mathbf{F}||^2$, $\forall \sigma > 0$, and for $\sigma = \sqrt{\alpha}/2$ we get

$$-\varepsilon w' + \sqrt{\alpha}w \leq \frac{4}{\sqrt{\alpha}}||\mathbf{F}||^2, \ w(x) \to 0, \ x \to \infty.$$

Reasoning from the contrary, we obtain that if for some continuously differentiable function $\Psi(x)$ following conditions are satisfied

$$\varepsilon\Psi' - \sqrt{\alpha}\Psi(x) \leq 0, \ x \geq L, \ \lim_{x \to \infty} \Psi(x) \geq 0, \tag{7}$$

then $\Psi(x) \geq 0$ for all $x \geq L$.

For $x \geq L$ we define

$$\Psi(x) = \frac{4}{\alpha} \max_{x \geq L} ||\mathbf{F}(x)||^2 - w(x).$$

Then the conditions (7) are satisfied and therefore $\Psi(x) \geq 0$, $x \geq L$, which proves the lemma.

Now we define the Cauchy problem with respect to the extracted variety (4):

$$\varepsilon \mathbf{W}'(x) + G(x)\mathbf{W}(x) = \beta(x), \ \mathbf{W}(0) = \mathbf{A}. \tag{8}$$

By analogy with lemma 4, we can prove the following lemma.

Lemma 5 *The following estimate of stability is true*

$$\max_x ||\mathbf{W}(x)|| \leq \sqrt{\frac{1}{\alpha^2} \max_x ||\beta(x)||^2 + ||\mathbf{A}||^2}. \tag{9}$$

Let us prove that the equation (4) extracts the variety of solutions of the equation (1) tending to zero at infinity.

Lemma 6 *Let $\mathbf{W}(x)$ be the solution of the problem (8), $G(x) \geq \sqrt{\alpha}I, \beta(x) \to \mathbf{0}$, $x \to \infty$. Then $\mathbf{W}(x) \to \mathbf{0}$, $x \to \infty$.*

Proof. Consider the problem

$$\varepsilon \mathbf{V}'(x) + \alpha \mathbf{V}(x) = \beta(x), \ \mathbf{V}(0) = \mathbf{A}.$$

For each component $V_i(x)$ we get

$$V_i(x) = A_i e^{-\alpha \varepsilon^{-1} x} + \frac{1}{\varepsilon} \int_0^x e^{-\alpha \varepsilon^{-1}(s-x)} \beta_i(s) d\,s.$$

Considering that $\beta_i(s) \to 0$, $s \to \infty$, from the last relation it is easy to get that $V_i(x) \to 0$ if $x \to \infty$, for any i. Therefore, $\mathbf{V}(x) \to \mathbf{0}$, for $x \to \infty$. Let $\mathbf{Z}(x) = \mathbf{V}(x) - \mathbf{W}(x)$. Then $\mathbf{Z}(x)$ is the solution of the problem

$$\varepsilon \mathbf{Z}'(x) + \alpha \mathbf{Z}(x) = (G(x) - \alpha I)\mathbf{W}(x), \ \mathbf{Z}(0) = \mathbf{0}.$$

Let $w = (\mathbf{Z}, \mathbf{Z})$. We multiply each term of the last equation by $\mathbf{Z}(x)$ and get

$$\frac{\varepsilon}{2} w' + \alpha w = ((G - \alpha I)\mathbf{W}, \mathbf{V}) - ((G - \alpha I)\mathbf{W}, \mathbf{W}) \leq ||(G - \alpha I)\mathbf{W}|| \, ||\mathbf{V}||.$$

Let $\Upsilon(x) = ||(G - \alpha I)\mathbf{W}(x)|| \, ||\mathbf{V}(x)||$. Then we come to the inequality

$$\frac{\varepsilon}{2} w'(x) + \alpha w(x) \leq \Upsilon(x). \tag{10}$$

We account that $\mathbf{W}(x)$ is bounded and $\mathbf{V}(x) \to \mathbf{0}$, $x \to \infty$. Then we obtain $\Upsilon(x) \to \mathbf{0}$, $x \to \infty$. Transforming inequality (10) and integrating from 0 up x, we obtain

$$w(x) \leq \frac{2}{\varepsilon} \int_0^x \Upsilon(s) e^{2\alpha \varepsilon^{-1}(s-x)} d\,s.$$

It is easy to conclude that $w(x) \to 0$, $x \to \infty$. Therefore, $\mathbf{Z}(x) \to \mathbf{0}$ if $x \to \infty$. This proves the lemma.

Using (4), we transform the problem (1)-(2) to the problem for a finite interval $[0, L]$:

$$\varepsilon^2 \mathbf{V}''(x) - P(x)\mathbf{V}(x) = \mathbf{F}(x), \ 0 < x < L, \tag{11}$$

$$\mathbf{V}(0) = \mathbf{A}, \ \varepsilon \mathbf{V}'(L) + G(L)\mathbf{V}(L) = \beta(L). \tag{12}$$

Lemma 7 *For the solution of the problem (11) - (12) the following estimate is true*

$$\max_{0 \le x \le L} ||\mathbf{V}(x)|| \le \sqrt{\frac{1}{\alpha^2} \max\{\max_x ||\mathbf{F}(x)||^2, \, ||\beta(L)||^2\} + ||\mathbf{A}||^2}. \tag{13}$$

Lemma 8 *Solutions of the problems (1)-(2) and (11) -(12) coincide on the interval $[0, L]$.*

Proof. For each of the considered problems the estimates of stability (3), (9), (13) are true, respectively. The stability estimates correspond to the uniqueness of the solution of the problems under consideration.

Let $\mathbf{W}(x)$ be the solution of the problem (8). Now we prove that $\mathbf{W}(x)$ is a solution of the problem (1)-(2). In accordance with lemma 6, the limit boundary condition (2) is satisfied for the function $\mathbf{W}(x)$. The equation (1) is satisfied by $\mathbf{W}(x)$ according to the choice of the matrix $G(x)$ and the vector function $\beta(x)$. So, $\mathbf{W}(x)$ is a solution of the problem (1)-(2). Similarly, we can verify that $\mathbf{W}(x)$ is solution of the problem (11)-(12) with $x \le L$. It proves the lemma.

In accordance with lemma 8, the problem (1)-(2) can be exactly transformed to the problem on a finite interval:

$$\varepsilon^2 \mathbf{U}''(x) - P(x)\mathbf{U}(x) = \mathbf{F}(x), \ 0 < x < L, \tag{14}$$

$$\mathbf{U}(0) = \mathbf{A}, \ \varepsilon \mathbf{U}'(L) + G(L)\mathbf{U}(L) = \beta(L). \tag{15}$$

Now we investigate the stability of the problem (14)-(15) to perturbation of the coefficients $G(L)$ and $\beta(L)$, which can be calculated only approximately.

Theorem 1 *Let $\tilde{\mathbf{U}}(x)$ be the solution of the problem (14)-(15) in the case when $G(L), \beta(L)$ are replaced by $\tilde{G}(L), \ \tilde{\beta}(L)$. Suppose that*

$$||G(L) - \tilde{G}(L)|| \le \Delta, \ ||\beta(L) - \tilde{\beta}(L)|| \le \Delta.$$

Then for some constant C

$$\max_x ||\mathbf{U}(x) - \tilde{\mathbf{U}}(x)|| \le C\Delta \exp\left[\sqrt{\alpha}(2\varepsilon)^{-1}(x - L)\right]. \tag{16}$$

Proof. Let $\mathbf{Z}(x) = \mathbf{U}(x) - \tilde{\mathbf{U}}(x)$. Then $\mathbf{Z}(x)$ is the solution of the problem:

$$\varepsilon^2 \mathbf{Z}''(x) - P(x)\mathbf{Z}(x) = \mathbf{0}, \quad \mathbf{Z}(0) = \mathbf{0}, \ \varepsilon \mathbf{Z}'(L) + G(L)\mathbf{Z}(L) = \mathbf{R}(L),$$

where $\mathbf{R}(L) = [\tilde{G}(L) - G(L)]\tilde{\mathbf{U}}(L) + \beta(L) - \tilde{\beta}(L)$. Multiplying this equations by $\mathbf{Z}$ and assuming $w(x) = ||\mathbf{Z}(x)||^2$, we obtain

$$\frac{\varepsilon^2}{2} w''(x) - \alpha w(x) \ge 0, \quad w(0) = 0, \ \varepsilon w'(L) + \sqrt{\alpha} w(L) \le \frac{1}{\sqrt{\alpha}} ||\mathbf{R}(L)||^2.$$

Define

$$\Psi(x) = \frac{1}{2\alpha} ||\mathbf{R}(L)||^2 \exp\left[\sqrt{\alpha}\varepsilon^{-1}(x - L)\right] - w(x).$$

Then

$$\frac{\varepsilon^2}{2} \Psi''(x) - \alpha \Psi(x) \le 0, \ x \in (0, L), \quad \Psi(0) \ge 0, \varepsilon\Psi'(L) + \sqrt{\alpha}\Psi(L) \ge 0.$$

From the fulfillment of these relations it follows that $\Psi(x) \ge 0$ for all x. This proves (16) with $C = (||\tilde{\mathbf{U}}(L)|| + 1)/\sqrt{2\alpha}$. The theorem is proven.

So, by (14)-(15) the problem (1)-(2) is precisely transformed to a finite interval. It remains to find the coefficients $G(L)$ and $\beta(L)$ from corresponding singular Cauchy problems. We'll find these coefficients by the expansion in the series [3], [4].

Expansions in powers of ε. Let

$$G^m(x) = \sum_{k=0}^{m} G_k(x)\varepsilon^k, \quad \beta^m(x) = \sum_{k=0}^{m} \beta_k(x)\varepsilon^k. \tag{17}$$

Substituting $G^m(x), \beta^m(x)$ into the equations (5), (6), we get recurrent formulas

$$G_0(x)G_k(x) + G_k(x)G_0(x) = G'_{k-1}(x) - \sum_{i=1}^{k-1} G_i(x)G_{k-i}(x), \ G_0(x) = \sqrt{P(x)};$$

$$G_0(x)\beta_k(x) = \beta'_{k-1}(x) - \sum_{i=1}^{k} G_i(x)\beta_{k-i}(x), \ k \geq 1, \ G_0(x)\beta_0(x) = -F(x).$$

It is easy to verify that the asymptotic approximation of $G(x)$ in (17) is the solution of the problem (5) with the perturbed matrix $\tilde{P}(x)$, similarly $\beta^m(x)$ is the solution of problem (6) with the perturbed vector function $\tilde{\mathbf{F}}(x)$, with the error of order $O(\varepsilon^{m+1})$.

Expansions in powers of x^{-1}. Applying such approach, we don't require the smallness of ε. May be $\varepsilon = 1$. Suppose that in (1) for $x \geq L$ the following decomposition is valid

$$P^m(x) = \sum_{k=0}^{m} \frac{P_k}{x^k}, \quad F^m(x) = \sum_{k=1}^{m} \frac{F_k}{x^k}.$$

Functions $G(x)$ and $\beta(x)$ will be searched as

$$G^m(x) = \sum_{k=0}^{m} \frac{G_k}{x^k}, \quad \beta^m(x) = \sum_{k=0}^{m} \frac{\beta_k}{x^k}.$$

Substituting these expansion into the matrix equation (5) and equating the coefficients with the same powers x, we get the recurrence formula:

$$G_0 G_k + G_k G_0 = P_k - (k-1)\varepsilon G_{k-1} - \sum_{i=1}^{k-1} G_i G_{k-i}, \quad G_0 = \sqrt{P_0}.$$

Let us construct the solution of the problem (6). Using the decomposition for $G(x)$, we get the recurrence formula

$$-G_0 \beta_k = (k-1)\varepsilon \beta_{k-1} + \sum_{i=1}^{k-1} G_i \beta_{k-i} + F_k, \ m \geq k \geq 1, \ \beta_0 = \mathbf{0}.$$

Then valid error estimates are

$$||G^m(x) - G(x)|| \leq CL^{-(m+1)}, \quad ||\beta^m(x) - \beta(x)|| \leq CL^{-(m+1)}, \quad x \geq L.$$

To find $G(x)$ based on asymptotic expansions it is required to solve the matrix equation $AX + XB = F$. Such methods were investigated in [7] and in other works.

So, the coefficients $G(L)$ and $\beta(L)$ for the problem (14)-(15) can be found with some given accuracy. In accordance with theorem 1, the solution of reduced problem is stable to arising errors.

3.   Error estimation of classical artificial boundary condition

In a number of papers, the boundary condition is transferred from infinity to the point L in the form $\mathbf{U}(L) = \mathbf{0}$. Let us estimate the error of such a transfer.

Let us move from the problem (1)-(2) to the problem:

$$\varepsilon^2 \tilde{\mathbf{U}}''(x) - P(x)\tilde{\mathbf{U}}(x) = \mathbf{F}(x), \quad \tilde{\mathbf{U}}(0) = \mathbf{A}, \quad \tilde{\mathbf{U}}(L) = \mathbf{0}. \tag{18}$$

Lemma 9 *For all $x \leq L$*

$$||\tilde{\mathbf{U}}(x) - \mathbf{U}(x)|| \leq ||\mathbf{U}(L)|| \exp\left[(\alpha/2)^{1/2}\varepsilon^{-1}(x - L)\right].$$

Proof. Let us $\mathbf{Z} = \mathbf{U} - \tilde{\mathbf{U}}$. Then $\mathbf{Z}(x)$ is the solution to the problem

$$\varepsilon^2 \mathbf{Z}''(x) - P(x)\mathbf{Z}(x) = \mathbf{0}, \quad \mathbf{Z}(0) = \mathbf{0}, \quad \mathbf{Z}(L) = \mathbf{U}(L).$$

Multiplying the equation and the boundary conditions scalarly by $\mathbf{Z}(x)$, we obtain relations for the scalar function $w(x) = (\mathbf{Z}(x), \mathbf{Z}(x))$:

$$\frac{\varepsilon^2}{2}w''(x) - \alpha w(x) \geq 0, \ w(0) = 0, \ w(L) = ||\mathbf{U}(L)||^2.$$

Now we define

$$\Psi(x) = ||\mathbf{U}(L)||^2 \exp\left[(2\alpha)^{1/2}\varepsilon^{-1}(x - L)\right] - w(x).$$

Then

$$\frac{\varepsilon^2}{2}\Psi''(x) - \alpha\Psi(x) \leq 0, \Psi(0) \geq 0, \ \Psi(L) \geq 0.$$

It follows from the fulfillment of these conditions that $\Psi(x) \geq 0$ for all $x \in [0, L]$. This proves the lemma.

According to the lemma, the error decreases exponentially with decreasing x.

4. Parabolic equation on the half-axis

Consider the problem for a parabolic equation

$$-\frac{\partial u}{\partial t} + \varepsilon^2 \frac{\partial^2 u}{\partial x^2} - b(x,t)u = f(x,t), \tag{19}$$

$$u(0,t) = \phi_1(t), u(x,0) = \phi_2(x), \lim_{x \to +\infty} u(x,t) = 0 \tag{20}$$

in unbounded domain $G = \{0 \leq x < \infty, 0 \leq t \leq T\}$. Functions b, f, ϕ_1, ϕ_2, are smooth enough and consistent so that the solution $u(x,t)$ is a twice continuously differentiable function in all interior points of the area G. We suppose that

$$\varepsilon > 0, \ b(x,t) \geq \gamma > 0, \lim_{x \to +\infty} \phi_2(x) = 0, \ \lim_{x \to +\infty} f(x,t) = 0. \tag{21}$$

Then the estimate $\max|u(x,t)| \leq \max|f(x,t)|/\gamma + \max|\phi_1(t)| + \max|\phi_2(x)|$ is true.

We approximate the equation (19) with the step τ in time

$$-\frac{u^i(x) - u^{i-1}(x)}{\tau} + \varepsilon^2 \frac{d^2 u^i}{d x^2} - b(x,t_i)u^i = f(x,t_i) \tag{22}$$

$$u^i(0) = \phi_1(t_i), u^0(x) = \phi_2(x), \lim_{x \to \infty} u^i(x) = 0, \tag{23}$$

where $t_i = \tau i, i = 1, 2, \ldots, M, t_M = T$. We have the estimate of accuracy

$$\max_{i,x} |u(x, t_i) - u^i(x)| \leq C\tau. \tag{24}$$

The problem (22)-(23) can be written in the form (1)-(2), while

$$U_i(x) = u^i(x), \ A_i = \phi_1(t_i), 1 \leq i \leq M, \ F_1(x) = f(x, t_1) + \frac{\phi_2(x)}{\tau},$$

$F_i(x) = f(x, t_i), 2 \leq i \leq M$, matrix $P(x)$ is following

$$P(x) = \begin{pmatrix} b(x, t_1) + \frac{1}{\tau} & 0 & \ldots & 0 \\ -\frac{1}{\tau} & b(x, t_2) + \frac{1}{\tau} & \ldots & 0 \\ & & \ldots & \\ 0 & \ldots & -\frac{1}{\tau} & b(x, t_M) + \frac{1}{\tau} \end{pmatrix}. \tag{25}$$

Further, on the basis of the developed approach the problem (22)-(23) can be reduced to a problem of the form (14)-(15) for a finite interval.

The reduced problem can be written as

$$-\frac{u^i(x) - u^{i-1}(x)}{\tau} + \varepsilon^2 \frac{d^2 u^i}{d x^2} - b(x, t_i)u^i = f(x, t_i), \ \ u^0(x) = \phi_2(x), \ 1 \leq i \leq M,$$

$$u^i(0) = \phi_1(t_i), \ \varepsilon \frac{d}{d x}u^i(L) + G_{i,i}u^i(L) = \beta_i(L) - \sum_{j=1}^{i-1} G_{i,j}(L)u^j(L). \tag{26}$$

According to (24) by (26) the problem (19)-(20) reduced to a finite interval with the error of order $O(\tau)$.

The matrix $P(x)$ from (25) is a diagonally dominant M-matrix, and therefore is positive-definite. Consequently, the obtained estimates of the errors that arise when the problem is set on a finite interval are also valid in the case of the problem (26).

In the problem (26) it remains to replace the derivative $(u^i)''(x)$ using a finite-difference relation and on each i-th level in time to solve the system of linear equations.

From the analysis of the problem (5) with $P(x)$ from (25) it follows that the matrix $G(x)$ is lower triangular. In this case the matrix equation $AX + XB = F$, arising in the construction of an asymptotic solution, can be solved explicitly:

$$X_{i,i-p} = \left[F_{i,i-p} - \sum_{k=i-p}^{i-1} A_{i,k}X_{k,i-p} - \sum_{k=i+1-p}^{i} X_{i,k}B_{k,i-p} \right] / [A_{i,i} + B_{i-p,i-p}], \tag{27}$$

where $p = 0, 1, 2, \ldots, i - 1$ and $i = 1, 2, \ldots, n$.

To use recurrent formulas for decomposition (17) we need to calculate the matrix root $G_0(x) = \sqrt{P(x)}$. Such methods were investigated, for example, in [8], [9]. Taking into account that matrix $P(x)$ is lower triangular, we can write an exact formula to find $X = \sqrt{P}$. For an arbitrary element $P_{i,i-p}$, with $p = 0, 1, 2, \ldots, i - 1$ can be written

$$\sum_{k=i-p}^{i} X_{i,k}X_{k,i-p} = P_{i,i-p}.$$

Then we get

$$X_{i,i-p} = \left[P_{i,i-p} - \sum_{k=i+1-p}^{i-1} X_{i,k}X_{k,i-p} \right] [X_{i,i} + X_{i-p,i-p}]^{-1}, \tag{28}$$

where

$$p = 1, 2, \ldots, i - 1, \quad x_{i,i} = \sqrt{P_{i,i}}, \quad 1 \le i \le M.$$

Note that the dimension of the matrix $P(x)$ increases with decreasing step τ.. Therefore, explicit formulas (27) and (28) are useful for solving the matrix equation and calculating the root of the matrix. In the future, it is intended to conduct computational experiments to verify the effectiveness of the approach under study.

Solutions of problems (1)-(2) and (19)-(20) have large gradients in the boundary layers near the point $x = 0$ if $\varepsilon \ll 1$. To achieve ε-uniform convergence of the difference scheme, one can use the mesh that condenses in the boundary layer, for example, Shishkin mesh [1].

5. Conclusion

In the work is investigated the method to transform a system of diffusion-reaction equations with a limit boundary condition at infinity to a problem for a finite interval. The reduced problem can be solved numerically by the application of a difference scheme. The method uses the well known approach based on the extraction of a stable variety of solutions that satisfy the limit condition at infinity. It is proposed to apply asymptotic expansions in a small parameter or x^{-1} to solve auxiliary Cauchy problems. The accuracy of such approach is estimated. It is shown how the approach can be applied to the numerical solution of a parabolic equation with the limit condition at infinity.

Acknowledgments

References

[1] Miller J J, O'Riordan E and Shishkin G I 1996 *Fitted Numerical Methods for Singular Perturbation Problems* (Singapore:World Scientific)
[2] Abramov A A 1962 On the transfer of the condition of boundedness for some systems of ordinary linear differential equations *U.S.S.R. Comput. Math. Math. Phys.* **1** 875-881
[3] Abramov A A, Konyukhova N B 1986 Transfer of admissible boundary conditions from a singular point of linear ordinary differential equations *Sov. J. Numer. Anal. Math. Modelling* **1** 245-265
[4] Abramov A A, Balla K, Konyukhova N B 1981 Transfer of boundary conditions from singular points for systems of ordinary differential equations *Reports on computing mathematics* (Moscow: Computing Centre of Academy of Sciences USSR)
[5] Zadorin A I Harina O V 2004 Numerical method for a system of linear equations of second order with a small parameter on a semi-infinite interval *Siberian J. of Numer. Mathematics* **7** 103-114
[6] Royden H L 1988 Comparison theorems for the matrix Riccati equation *Communs Pure and Appl. Math.* **41** 739-746
[7] Ikramov Kh D 1984 *Numerical solution of matrix equations* (Moscow: Nauka)
[8] Alefeld G, Schneider N 1982 On squre roots of M-matrices *Linear algebra and its applications* **42** 119-132
[9] Long J-h 2008 Newton's method with exact line search for the square root of a matrix *J. Phys. Conf. Ser.* **96** 012034