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# A probabilistic approach to the solution of the Neumann problem for nonlinear parabolic equations

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AND

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A number of new layer methods for solving the Neumann problem for semilinear parabolic equations are constructed by using probabilistic representations of their solutions. The methods exploit the ideas of weak-sense numerical integration of stochastic differential equations in a bounded domain. In spite of the probabilistic nature these methods are nevertheless deterministic. Some convergence theorems are proved. Numerical tests on the Burgers equation are presented.

*Keywords*: Numerical methods for parabolic equations; probabilistic representations; weak approximation of stochastic differential equations.

## 1. Introduction

A probabilistic approach to constructing layer methods for solving nonlinear partial differential equations (PDEs) of parabolic type is proposed in Milstein (1997), Milstein & Tretyakov (2000a) and Milstein & Tretyakov (2001). The papers Milstein (1997) and Milstein & Tretyakov (2000a) are devoted to layer approximation methods for the Cauchy problem for semilinear parabolic equations and the paper Milstein & Tretyakov (2001) deals with the nonlinear Dirichlet problem. The aim of the present paper is to develop such methods for nonlinear problems with Neumann boundary conditions.

Let G be a bounded domain in  $\mathbf{R}^d$ ,  $Q = [t_0, T) \times G$  be a cylinder in  $\mathbf{R}^{d+1}$ ,  $\Gamma = \overline{Q} \setminus Q$ . The set  $\Gamma$  is a part of the boundary of the cylinder Q consisting of the upper base and the lateral surface. Consider the Neumann problem for the semilinear parabolic

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equation

$$\frac{\partial u}{\partial t} + \frac{1}{2} \sum_{i,j=1}^{d} a^{ij}(t,x,u) \frac{\partial^2 u}{\partial x^i \partial x^j} + \sum_{i=1}^{d} b^i(t,x,u) \frac{\partial u}{\partial x^i} + g(t,x,u) = 0, \ (t,x) \in Q,$$
(1.1)

with the initial condition

$$u(T, x) = \varphi(x) \tag{1.2}$$

and the boundary condition

$$\frac{\partial u}{\partial v} = \psi(t, x, u), \ t \in [t_0, T], \ x \in \partial G,$$
(1.3)

where v is the direction of the internal normal to the boundary  $\partial G$  at the point  $x \in \partial G$ .

The form of (1.1) is relevant to a probabilistic approach, i.e. the equation is considered under t < T, and the 'initial' condition is prescribed at t = T. Using the well known probabilistic representation of the solution to (1.1)–(1.3) (see Gichman & Skorochod (1972), Freidlin (1985)), we get

$$u(t, x) = \mathbf{E}(\varphi(X_{t,x}(T)) + Z_{t,x,0}(T)),$$
(1.4)

where  $X_{t,x}(s)$ ,  $Z_{t,x,z}(s)$ ,  $t_0 \le t < T$ ,  $s \ge t$ ,  $x \in \overline{G}$ , is a solution of the Cauchy problem to the Ito system of stochastic differential equations (SDEs)

$$dX = b(s, X, u(s, X))I_G(X)ds + \sigma(s, X, u(s, X))I_G(X)dw(s) + v(X)I_{\partial G}(X)d\mu(s), \quad X(t) = x, dZ = g(s, X, u(s, X))I_G(X)ds + \psi(s, X, u(s, X))I_{\partial G}(X)d\mu(s), \quad Z(t) = z.$$
(1.5)

Here  $w(s) = (w^1(s), \dots, w^d(s))^\top$  is a standard Wiener process,  $b(s, x, u) = (b^1(s, x, u), \dots, b^d(s, x, u))^\top$  is a column vector, the matrix  $\sigma = \sigma(s, x, u)$  is obtained from the equation

$$\sigma\sigma^{\top} = a, \ \sigma = \{\sigma^{ij}(s, x, u)\}, \ a = \{a^{ij}(s, x, u)\}, \ i, j = 1, \dots, d,$$

 $\mu(s)$  is a local time of the process X on  $\partial G$ , and  $I_A(x)$  is the indicator of a set A.

We recall that the local time is a continuous, nondecreasing random process which increases only on the set  $\{t \ge t_0, X_{t_0,x}(t) \in \partial G\}$ . The Lebesgue measure of this set is zero. A tutorial on processes with reflection is available in, for example, Freidlin (1985, Section 1.6).

Introduce a time discretization, for definiteness the equidistant one:

$$T = t_N > t_{N-1} > \cdots > t_0, \ h := \frac{T - t_0}{N}.$$

The methods proposed here give an approximation  $\overline{u}(t_k, x)$  of the solution  $u(t_k, x)$ ,  $k = N, \ldots, 0, x \in \overline{G}$ , i.e. step by step everywhere in the domain  $\overline{G}$ . They exploit the

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ideas of weak-sense numerical integration of SDEs in a bounded domain from Milstein (1995b, 1996). As a result, we express  $\bar{u}(t_k, x)$  recurrently in terms of  $\bar{u}(t_{k+1}, x)$ ,  $k = N - 1, \ldots, 0$ , i.e. we construct some layer methods which are discrete in the variable *t* only. In spite of their probabilistic nature these methods are nevertheless deterministic.

Let us note that finite-difference methods also express an approximate solution on the layer  $t = t_k$  recurrently in terms of the solution on the layer  $t = t_{k+1}$ . For their construction, both the time step  $\Delta t$  and the space step  $\Delta x$  are used. Moreover, the knots of the layer  $t = t_{k+1}$  used to evaluate  $\bar{u}(t_k, x_j)$  are definitely prescribed. In our methods we use the time step h only, and the points from the layer  $t = t_{k+1}$  to evaluate  $\bar{u}(t_k, x)$  arise automatically. A location of these points depends on the coefficients of the problem considered and on the weak scheme chosen. As a result, the probabilistic approach takes into account a coefficient dependence on the space variables and a relationship between diffusion and advection in an intrinsic manner. In particular, it was demonstrated in numerical tests (see Milstein & Tretyakov (2001) and Section 7.2 of this paper) that layer methods may be preferable to finite-difference ones in the case of strong advection. We should also note that the probabilistic approach gives a natural way to derive many various new methods.

In Section 2, two layer methods for the nonlinear Neumann problem are constructed. Using probabilistic-type arguments, a convergence theorem is proved in Section 3. To realize a layer method in practice, a discretization in the variable x with interpolation at every step is needed to turn the method into an algorithm. Such numerical algorithms are given in Section 4. A majority of ideas can be demonstrated at d = 1, and we restrict ourselves to this case in Sections 2–4. The case  $d \ge 2$  is discussed in Section 5. Two additional layer methods are proposed in Section 6. Numerical tests are presented in the last section. Their results are in complete agreement with theoretical ones.

Traditional numerical analysis of nonlinear PDEs is available, for example in Quarteroni & Valli (1994), Samarskii (1977), Strikwerda (1989) and Vreugdenhil & Koren (1993). The probabilistic approach to boundary value problems for linear parabolic equations is treated in Milstein (1995a,b, 1996) and Costantini *et al.* (1998). Other probabilistic approaches are considered in Kushner (1977) and Talay & Tubaro (1996).

#### 2. Construction of layer methods

The Neumann boundary value problem in the one-dimensional case has the form

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sigma^2(t, x, u)\frac{\partial^2 u}{\partial x^2} + b(t, x, u)\frac{\partial u}{\partial x} + g(t, x, u) = 0, \quad t_0 \le t < T, \ \alpha < x < \beta,$$
(2.1)

$$u(T, x) = \varphi(x), \ \alpha \leqslant x \leqslant \beta; \tag{2.2}$$

$$\frac{\partial u}{\partial x}(t,\alpha) = \psi_1(t,u(t,\alpha)), \quad \frac{\partial u}{\partial x}(t,\beta) = \psi_2(t,u(t,\beta)), \quad t_0 \le t \le T.$$
(2.3)

In this case *Q* is a partly open rectangle:  $Q = [t_0, T) \times (\alpha, \beta)$ , and  $\Gamma$  consists of the upper base  $\{T\} \times [\alpha, \beta]$  and two vertical intervals:  $[t_0, T) \times \{\alpha\}$  and  $[t_0, T) \times \{\beta\}$ . We assume that  $\sigma(t, x, u) \ge \sigma_* > 0$  for  $(t, x) \in \overline{Q}$ ,  $-\infty < u < \infty$ .

Let u = u(t, x) be a solution to the problem (2.1)–(2.3) which is supposed to exist, to be unique, and to be sufficiently smooth. Theoretical results on this topic are available in Ladyzhenskaya *et al.* (1988) and Taylor (1996) (see also references therein).

Analogously to (1.4), we have the local representation

$$u(t_k, x) = \mathbf{E}(u(t_{k+1}, X_{t_k, x}(t_{k+1})) + Z_{t_k, x, 0}(t_{k+1})),$$
(2.4)

where  $X_{t,x}(s)$ ,  $Z_{t,x,z}(s)$ ,  $t_0 \leq t < T$ ,  $s \geq t$ ,  $x \in [\alpha, \beta]$ , satisfy (1.5).

Applying a slightly modified weak scheme with one-step boundary order  $O(h^{3/2})$  from Milstein (1995b, 1996) to system (1.5), it is not difficult to obtain

$$\begin{aligned} X_{t_k,x}(t_{k+1}) \simeq \bar{X}_{t_k,x}(t_{k+1}) &= x + h\tilde{b}_k + h^{1/2}\tilde{\sigma}_k\xi_k, \\ Z_{t_k,x,z}(t_{k+1}) \simeq \bar{Z}_{t_k,x,z}(t_{k+1}) &= z + h\tilde{g}_k, \quad \text{if } x + h\tilde{b}_k \pm h^{1/2}\tilde{\sigma}_k \in [\alpha,\beta]; \\ \bar{X}_{t_k,x}(t_{k+1}) &= x + (\alpha - x) + \sqrt{h\tilde{\sigma}_k^2 + (\alpha - x)^2}, \\ \bar{Z}_{t_k,x,z}(t_{k+1}) &= z + h\tilde{g}_k - \psi_1(t_k, u(t_k,\alpha)) \cdot (\alpha - x - h\tilde{b}_k + \sqrt{h\tilde{\sigma}_k^2 + (\alpha - x)^2}), \\ &\quad \text{if } x + h\tilde{b}_k - h^{1/2}\tilde{\sigma}_k < \alpha; \\ \bar{X}_{t_k,x}(t_{k+1}) &= x + (\beta - x) - \sqrt{h\tilde{\sigma}_k^2 + (\beta - x)^2}, \\ \bar{Z}_{t_k,x,z}(t_{k+1}) &= z + h\tilde{g}_k - \psi_2(t_k, u(t_k,\beta)) \cdot (\beta - x - h\tilde{b}_k - \sqrt{h\tilde{\sigma}_k^2 + (\beta - x)^2}), \\ &\quad \text{if } x + h\tilde{b}_k + h^{1/2}\tilde{\sigma}_k > \beta. \end{aligned}$$

$$(2.5)$$

Here  $\tilde{b}_k$ ,  $\tilde{\sigma}_k$ ,  $\tilde{g}_k$  are the coefficients b(t, x, u),  $\sigma(t, x, u)$ , g(t, x, u) calculated at the point  $(t_k, x, u(t_k, x))$  and  $\xi_{N-1}, \xi_{N-2}, \ldots, \xi_0$  are i.i.d. random variables with the law  $P(\xi = \pm 1) = 1/2$ .

One can see that using approximation (2.5) and representation (2.4), we get an implicit one-step approximation for  $u(t_k, x)$ . Applying the method of simple iteration to this implicit approximation with  $u(t_{k+1}, x)$  as a null iteration, we come to the explicit one-step approximation  $v(t_k, x)$  of  $u(t_k, x)$ :

$$v(t_{k}, x) = \frac{1}{2}u(t_{k+1}, x + hb_{k} - h^{1/2}\sigma_{k}) + \frac{1}{2}u(t_{k+1}, x + hb_{k} + h^{1/2}\sigma_{k}) + hg_{k},$$
  
if  $x + hb_{k} \pm h^{1/2}\sigma_{k} \in [\alpha, \beta];$   
 $v(t_{k}, x) = u(t_{k+1}, \alpha + \sqrt{h\sigma_{k}^{2} + (\alpha - x)^{2}})$   
 $-\psi_{1}(t_{k+1}, u(t_{k+1}, \alpha)) \cdot (\alpha - x - hb_{k} + \sqrt{h\sigma_{k}^{2} + (\alpha - x)^{2}}) + hg_{k},$   
if  $x + hb_{k} - h^{1/2}\sigma_{k} < \alpha;$   
 $v(t_{k}, x) = u(t_{k+1}, \beta - \sqrt{h\sigma_{k}^{2} + (\beta - x)^{2}})$   
 $-\psi_{2}(t_{k+1}, u(t_{k+1}, \beta)) \cdot (\beta - x - hb_{k} - \sqrt{h\sigma_{k}^{2} + (\beta - x)^{2}}) + hg_{k},$   
if  $x + hb_{k} + h^{1/2}\sigma_{k} > \beta;$   
 $k = N - 1, \dots, 1, 0,$  (2.6)

where  $b_k$ ,  $\sigma_k$ ,  $g_k$  are the coefficients b,  $\sigma$ , g calculated at the point  $(t_k, x, u(t_{k+1}, x))$ . Let us observe that within the limits of the considered accuracy it is possible to take  $t_{k+1}$  instead of

 $t_k$ . That is why one can take, for instance,  $\psi_1(t_{k+1}, u(t_{k+1}, \alpha))$  instead of  $\psi_1(t_k, u(t_{k+1}, \alpha))$  in (2.6).

The corresponding explicit layer method for solving the Neumann problem (2.1)–(2.3) has the form

$$\begin{split} \bar{u}(t_N, x) &= \varphi(t_N, x), \ x \in [\alpha, \beta], \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \\ &\quad \text{if} \ x + h\bar{b}_k \pm h^{1/2}\bar{\sigma}_k \in [\alpha, \beta]; \\ \bar{u}(t_k, x) &= \bar{u}(t_{k+1}, \alpha + \sqrt{h\bar{\sigma}_k^2 + (\alpha - x)^2}) \\ -\psi_1(t_{k+1}, \bar{u}(t_{k+1}, \alpha)) \cdot (\alpha - x - h\bar{b}_k + \sqrt{h\bar{\sigma}_k^2 + (\alpha - x)^2}) + h\bar{g}_k, \\ &\quad \text{if} \ x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k < \alpha; \\ \bar{u}(t_k, x) &= \bar{u}(t_{k+1}, \beta - \sqrt{h\bar{\sigma}_k^2 + (\beta - x)^2}) \\ -\psi_2(t_{k+1}, \bar{u}(t_{k+1}, \beta)) \cdot (\beta - x - h\bar{b}_k - \sqrt{h\bar{\sigma}_k^2 + (\beta - x)^2}) + h\bar{g}_k, \\ &\quad \text{if} \ x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k > \beta; \\ &\quad k = N - 1, \dots, 1, 0, \end{split}$$
(2.7)

where  $\bar{b}_k = \bar{b}_k(x) = b(t_k, x, \bar{u}(t_{k+1}, x)), \, \bar{\sigma}_k = \bar{\sigma}_k(x) = \sigma(t_k, x, \bar{u}(t_{k+1}, x)), \, \bar{g}_k = \bar{g}_k(x)$ =  $g(t_k, x, \bar{u}(t_{k+1}, x)).$ 

This layer method has the one-step error near the boundary estimated by  $O(h^{3/2})$  and for internal points estimated by  $O(h^2)$  (see Lemma 3.1). We prove that its order of convergence is O(h) when the boundary condition does not depend on the solution (see Theorem 3.1). Apparently, this is so in the general case as well (see Remark 3.1).

Another method with the same one-step error is given in Section 6.

Applying the weak scheme with one-step boundary order O(h) from Milstein (1995b, 1996) to system (1.5), it is not difficult to obtain

$$\begin{split} X_{t_k,x}(t_{k+1}) &\simeq \bar{X}_{t_k,x}(t_{k+1}) = x + h\tilde{b}_k + h^{1/2}\tilde{\sigma}_k\xi_k, \\ Z_{t_k,x,z}(t_{k+1}) &\simeq Z_{t_k,x,z}(t_{k+1}) = z + h\tilde{g}_k, \text{ if } x + h\tilde{b}_k \pm h^{1/2}\tilde{\sigma}_k \in [\alpha,\beta]; \\ \bar{X}_{t_k,x}(t_{k+1}) &= x + qh^{1/2}, \ \bar{Z}_{t_k,x,z}(t_{k+1}) = z - \psi_1(t_k, u(t_k,\alpha))qh^{1/2}, \\ &\quad \text{if } x + h\tilde{b}_k - h^{1/2}\tilde{\sigma}_k < \alpha; \\ \bar{X}_{t_k,x}(t_{k+1}) &= x - qh^{1/2}, \ \bar{Z}_{t_k,x,z}(t_{k+1}) = z + \psi_2(t_k, u(t_k,\beta))qh^{1/2}, \\ &\quad \text{if } x + h\tilde{b}_k + h^{1/2}\tilde{\sigma}_k > \beta. \end{split}$$
(2.8)

Here  $\tilde{b}_k$ ,  $\tilde{\sigma}_k$ ,  $\tilde{g}_k$  are the coefficients b(t, x, u),  $\sigma(t, x, u)$ , g(t, x, u) calculated at the point  $(t_k, x, u(t_k, x)), \xi_{N-1}, \xi_{N-2}, \ldots, \xi_0$  are i.i.d. random variables with the law  $P(\xi = \pm 1) = 1/2$ , and q is a positive number (see Remark 3.2, where a discussion on choosing q is given). As before, we obtain the following explicit one-step approximation  $v(t_k, x)$  of

 $u(t_k, x)$ :

$$v(t_k, x) = \frac{1}{2}u(t_{k+1}, x + hb_k - h^{1/2}\sigma_k) + \frac{1}{2}u(t_{k+1}, x + hb_k + h^{1/2}\sigma_k) + hg_k,$$
  
if  $x + hb_k \pm h^{1/2}\sigma_k \in [\alpha, \beta];$   

$$v(t_k, x) = u(t_{k+1}, x + qh^{1/2}) - \psi_1(t_{k+1}, u(t_{k+1}, \alpha))qh^{1/2}, \text{ if } x + hb_k - h^{1/2}\sigma_k < \alpha;$$
  

$$v(t_k, x) = u(t_{k+1}, x - qh^{1/2}) + \psi_2(t_{k+1}, u(t_{k+1}, \beta))qh^{1/2}, \text{ if } x + hb_k + h^{1/2}\sigma_k > \beta;$$
  

$$k = N - 1, \dots, 1, 0.$$
(2.9)

The corresponding explicit layer method for solving the Neumann problem (2.1)–(2.3) has the form

$$\begin{split} \bar{u}(t_N, x) &= \varphi(t_N, x), \ x \in [\alpha, \beta], \\ \bar{u}(t_k, x) &= \frac{1}{2} \bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2} \bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \\ & \text{if} \ x + h\bar{b}_k \pm h^{1/2}\bar{\sigma}_k \in [\alpha, \beta]; \\ \bar{u}(t_k, x) &= \bar{u}(t_{k+1}, x + qh^{1/2}) - \psi_1(t_{k+1}, \bar{u}(t_{k+1}, \alpha))qh^{1/2}, \text{ if } x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k < \alpha; \\ \bar{u}(t_k, x) &= \bar{u}(t_{k+1}, x - qh^{1/2}) + \psi_2(t_{k+1}, \bar{u}(t_{k+1}, \beta))qh^{1/2}, \text{ if } x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k > \beta; \end{split}$$

 $k = N - 1, \dots, 1, 0,$  (2.10)

where  $\bar{b}_k = \bar{b}_k(x) = b(t_k, x, \bar{u}(t_{k+1}, x)), \, \bar{\sigma}_k = \bar{\sigma}_k(x) = \sigma(t_k, x, \bar{u}(t_{k+1}, x)), \, \bar{g}_k = \bar{g}_k(x)$ =  $g(t_k, x, \bar{u}(t_{k+1}, x)).$ 

This layer method is simpler but less accurate than (2.7). Its one-step error near the boundary is O(h) and for internal points is  $O(h^2)$  (see Lemma 3.3). We prove that its order of convergence is  $O(h^{1/2})$  when the boundary condition does not depend on the solution (see Theorem 3.2). Apparently, this is so in the general case as well.

A method of the same convergence order is proposed for the linear Neumann problem in Costantini *et al.* (1998). This method is extended to the nonlinear problem in Section 6.

## 3. Convergence theorems

We make the following assumptions.

(i) There exists a unique solution u(t, x) of the problem (2.1)–(2.3) such that

$$-\infty \leqslant u_{\circ} < u_{*} \leqslant u(t,x) \leqslant u^{*} < u^{\circ} \leqslant \infty, \ t_{0} \leqslant t \leqslant T, \ x \in [\alpha,\beta],$$
(3.1)

where  $u_{\circ}$ ,  $u_{*}$ ,  $u^{*}$ ,  $u^{\circ}$  are some constants, and there exist the uniformly bounded derivatives:

$$\left|\frac{\partial^{i+j}u}{\partial t^{i}\partial x^{j}}\right| \leqslant K, \ i = 0, \ j = 1, 2, 3, 4; \ i = 1, \ j = 0, 1, 2; \ i = 2, \ j = 0;$$
$$t_{0} \leqslant t \leqslant T, \ x \in [\alpha, \beta].$$
(3.2)

(ii) The coefficients b(t, x, u),  $\sigma(t, x, u)$ , g(t, x, u) are uniformly bounded and uniformly satisfy the Lipschitz condition with respect to x and u:

$$|b| \leq K, \ |\sigma| \leq K, \ |g| \leq K,$$
  

$$|b(t, x_2, u_2) - b(t, x_1, u_1)| + |\sigma(t, x_2, u_2) - \sigma(t, x_1, u_1)| + |g(t, x_2, u_2) - g(t, x_1, u_1)|$$
  

$$\leq K \left(|x_2 - x_1| + |u_2 - u_1|\right),$$
  

$$t_0 \leq t \leq T, \ x \in [\alpha, \beta], \ u_{\circ} < u < u^{\circ}.$$
  
(3.3)

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Below we use the letters K and C without any index for various constants which do not depend on h, k, x.

Let us evaluate the one-step error  $\rho(t_k, x)$  of method (2.7).

LEMMA 3.1 Under assumptions (i) and (ii), the one-step error  $\rho(t_k, x)$  of method (2.7) is estimated as

$$|\rho(t_k, x)| = |v(t_k, x) - u(t_k, x)| \le Ch^2, \ x + hb_k \pm h^{1/2}\sigma_k \in [\alpha, \beta];$$
(3.4)

$$|\rho(t_k, x)| = |v(t_k, x) - u(t_k, x)| \le Ch^{3/2}, \ x + hb_k - h^{1/2}\sigma_k < \alpha \text{ or } x + hb_k + h^{1/2}\sigma_k > \beta,$$
(3.5)

where  $v(t_k, x)$  is the corresponding one-step approximation, and *C* does not depend on *h*, *k*, *x*.

*Proof.* If both the points  $x + hb_k \pm h^{1/2}\sigma_k$  belong to  $[\alpha, \beta]$ , we have

$$v(t_k, x) = \frac{1}{2}u(t_{k+1}, x + hb_k - h^{1/2}\sigma_k) + \frac{1}{2}u(t_{k+1}, x + hb_k + h^{1/2}\sigma_k) + hg_k.$$
 (3.6)

Expanding the terms of (3.6) at the point  $(t_k, x)$  and taking into account that u(t, x) is the solution of problem (2.1)–(2.3), we get (3.4) (see also Milstein (1997), Milstein & Tretyakov (2000a), where similar assertions are proved in detail).

Let us consider the case when the point  $x + hb_k - h^{1/2}\sigma_k < \alpha$ . Due to (2.6), we get

$$v(t_k, x) = u(t_{k+1}, x + \Delta X^{\alpha}) - \psi_1(t_{k+1}, u(t_{k+1}, \alpha)) \cdot (\Delta X^{\alpha} - hb_k) + hg_k, \quad (3.7)$$

where

$$\Delta X^{\alpha} := \alpha - x + \sqrt{h\sigma_k^2 + (\alpha - x)^2}.$$

It is clear that

$$|\alpha - x| \leqslant Ch^{1/2}, \quad |\Delta X^{\alpha}| \leqslant Ch^{1/2}. \tag{3.8}$$

Taking into account that  $\psi_1(t_{k+1}, u(t_{k+1}, \alpha)) = u'_x(t_{k+1}, \alpha)$  (see (2.3)), then expanding the functions  $u(t_{k+1}, x + \Delta X^{\alpha})$  and  $u'_x(t_{k+1}, x + (\alpha - x))$  at the point  $(t_k, x)$ , and using assumptions (i), (ii), and inequalities (3.8), we get

$$v(t_k, x) = u + \frac{\partial u}{\partial t}h + \frac{\partial u}{\partial x}\Delta X^{\alpha} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}(\Delta X^{\alpha})^2 -\frac{\partial u}{\partial x}(\Delta X_{\alpha} - hb_k) - \frac{\partial^2 u}{\partial x^2}(\alpha - x)\Delta X^{\alpha} + g_k h + O(h^{3/2}) = u + h\left(\frac{\partial u}{\partial t} + b_k\frac{\partial u}{\partial x} + g_k\right) + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta X^{\alpha}(\Delta X^{\alpha} - 2(\alpha - x)) + O(h^{3/2}), \quad (3.9)$$

where the function *u* and its derivatives are calculated at the point  $(t_k, x)$ . The expression  $\Delta X^{\alpha} (\Delta X^{\alpha} - 2(\alpha - x))$  is equal to  $h\sigma_k^2$ .

Due to assumptions (i) and (ii), we obtain

$$b_k = b(t_k, x, u(t_{k+1}, x)) = \tilde{b}_k + O(h), \ \sigma_k^2 = \tilde{\sigma}_k^2 + O(h), \ g_k = \tilde{g}_k + O(h),$$

where  $\tilde{b}_k$ ,  $\tilde{\sigma}_k$ ,  $\tilde{g}_k$  are calculated at the point  $(t_k, x, u(t_k, x))$ . Then we get from (3.9):

$$v(t_k, x) = u + h\left(\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} + \frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2} + g\right) + O(h^{3/2}).$$
(3.10)

Since u(t, x) is the solution of problem (2.1)–(2.3), the relation (3.10) implies

$$v(t_k, x) = u(t_k, x) + O(h^{3/2}).$$

The case  $x + hb_k + h^{1/2}\sigma_k > \beta$  can be considered analogously.

To prove the theorem on global convergence for method (2.7), we need some auxiliary constructions. Let us introduce the random sequence  $X_i$ ,  $Z_i$ :

$$X_{k} = x, \ Z_{k} = 0,$$

$$X_{i+1} = X_{i} + h\check{b}_{i} + h^{1/2}\check{\sigma}_{i}\xi_{i}, \ Z_{i+1} = Z_{i} + h\check{g}_{i},$$
if  $X_{i} + h\check{b}_{i} \pm h^{1/2}\check{\sigma}_{i} \in [\alpha, \beta];$ 

$$X_{i+1} = X_{i} + \Delta X_{i}^{\alpha}, \ Z_{i+1} = Z_{i} + h\check{g}_{i} - \psi_{1}(t_{i+1}) \cdot (\Delta X_{i}^{\alpha} - h\check{b}_{i}),$$

$$\Delta X_{i}^{\alpha} := (\alpha - X_{i}) + \sqrt{h\check{\sigma}_{i}^{2} + (\alpha - X_{i})^{2}},$$
if  $X_{i} + h\check{b}_{i} - h^{1/2}\check{\sigma}_{i} < \alpha;$ 

$$X_{i+1} = X_{i} + \Delta X_{i}^{\beta}, \ Z_{i+1} = Z_{i} + h\check{g}_{i} - \psi_{2}(t_{i+1}) \cdot (\Delta X_{i}^{\beta} - h\check{b}_{i}),$$

$$\Delta X_{i}^{\beta} := (\beta - X_{i}) - \sqrt{h\check{\sigma}_{i}^{2} + (\beta - X_{i})^{2}},$$
if  $X_{i} + h\check{b}_{i} + h^{1/2}\check{\sigma}_{i} > \beta;$ 

$$i = k, \dots, N - 1, \ k \ge 0.$$
(3.11)

Here  $\xi_i$  are i.i.d. random variables with the law  $P(\xi = \pm 1) = \frac{1}{2}$  and  $\tilde{b}_i = \bar{b}_i(X_i) = b(t_i, X_i, \bar{u}(t_{i+1}, X_i))$ ,  $\check{\sigma}_i = \bar{\sigma}_i(X_i) = \sigma(t_i, X_i, \bar{u}(t_{i+1}, X_i))$ ,  $\check{g}_i = \bar{g}_i(X_i) = g(t_i, X_i, \bar{u}(t_{i+1}, X_i))$ . Let us note that the function  $\bar{u}(t_i, x)$ ,  $i = 0, \dots, N$ ,  $x \in [\alpha, \beta]$ , is uniquely defined by (2.7). Evidently, the sequence  $(t_i, X_i)$  is a Markov chain.

Introduce the boundary layer  $\partial \Gamma \in \overline{Q}$ : for all the points  $(t_k, x) \in \overline{Q} \setminus \partial \Gamma$ , both the points  $x + h\bar{b}_k(x) \pm h^{1/2}\bar{\sigma}_k(x)$  belong to  $[\alpha, \beta]$ , and for the points  $(t_k, x) \in \partial \Gamma$ , either  $x + h\bar{b}_k(x) - h^{1/2}\bar{\sigma}_k(x) \notin [\alpha, \beta]$  or  $x + h\bar{b}_k(x) + h^{1/2}\bar{\sigma}_k(x) \notin [\alpha, \beta]$ .

LEMMA 3.2 Under assumptions (i) and (ii), the mean number of steps  $\varkappa(t_k, x)$ , which the Markov chain  $(t_i, X_i)$ , i = k, ..., N,  $k \ge 0$ ,  $X_k = x$ , spends in the layer  $\partial \Gamma$ , is estimated as

$$E\varkappa(t_k, x) \leqslant \frac{C}{\sqrt{h}},$$

where C does not depend on h, k, x.

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The proof of Lemma 3.2 differs only little from the proof of the corresponding lemma on the mean number of steps in the case of the linear Neumann problem given in Milstein (1996) and is therefore omitted.

THEOREM 3.1 Let the Neumann problem for (2.1) with condition (2.2) have the following boundary conditions:

$$\frac{\partial u}{\partial x}(t,\alpha) = \psi_1(t), \quad \frac{\partial u}{\partial x}(t,\beta) = \psi_2(t), \quad t_0 \leqslant t \leqslant T.$$
(3.12)

Under assumptions (i) and (ii), the method (2.7) has the first order of convergence with respect to h, i.e.

$$|\bar{u}(t_k, x) - u(t_k, x)| \leq Kh,$$

where K does not depend on h, k, x.

*Proof.* Here we exploit ideas of proving convergence theorems for probabilistic methods from Milstein (1995a,b, 1996); Milstein & Tretyakov (2001).

Let  $X_i$ ,  $Z_i$ , i = k, ..., N,  $X_k = x$ ,  $Z_k = 0$ , be the sequence defined by (3.11). It is clear that

$$\bar{u}(t_k, x) = E\left[\bar{u}(t_N, X_N) + Z_N\right] = E\left[\varphi(t_N, X_N) + Z_N\right] = E\left[u(t_N, X_N) + Z_N\right].$$

Introduce the notation  $R(t_k, x) := \overline{u}(t_k, x) - u(t_k, x)$ . Then we get

$$R(t_k, x) = E [u(t_N, X_N) + Z_N] - u(t_k, x)$$
  
=  $\sum_{i=k}^{N-1} E [u(t_{i+1}, X_{i+1}) - u(t_i, X_i) + Z_{i+1} - Z_i]$   
=  $\sum_{i=k}^{N-1} E I_{\overline{Q} \setminus \partial \Gamma}(t_i, X_i) [u(t_{i+1}, X_{i+1}) - u(t_i, X_i) + Z_{i+1} - Z_i]$   
+  $\sum_{i=k}^{N-1} E I_{\partial \Gamma}(t_i, X_i) [u(t_{i+1}, X_{i+1}) - u(t_i, X_i) + Z_{i+1} - Z_i].$  (3.13)

Denote the first sum in the right-hand side of (3.13) by  $R^{(1)}(t_k, x)$  and the second one by  $R^{(2)}(t_k, x)$ .

Below we use the known properties of conditional expectations taking into account that the indicator functions  $I_{\overline{O}\setminus\partial\Gamma}$  and  $I_{\partial\Gamma}$  are measurable with respect to  $X_i$ . We have

$$R^{(1)}(t_k, x) = \sum_{i=k}^{N-1} E I_{\overline{Q} \setminus \partial \Gamma}(t_i, X_i) \left[ u(t_{i+1}, X_{i+1}) - u(t_i, X_i) + Z_{i+1} - Z_i \right]$$
(3.14)

$$= \sum_{i=k}^{N-1} E(I_{\overline{Q}\setminus\partial\Gamma}(t_i, X_i)E[u(t_{i+1}, X_{i+1}) - u(t_i, X_i) + Z_{i+1} - Z_i / X_i, Z_i]).$$

To calculate the conditional expectation in (3.14), we exploit a lemma from Gichman & Skorochod (1972, Section 10). The lemma allows us to evaluate a conditional expectation as the ordinary expectation under fixed values of the random variables  $X_i$ ,  $Z_i$ . According to (3.11), we obtain for  $(t_i, X_i) \in \overline{Q} \setminus \partial \Gamma$ :

$$A_{i} := E \left[ u(t_{i+1}, X_{i+1}) - u(t_{i}, X_{i}) + Z_{i+1} - Z_{i} \swarrow X_{i}, Z_{i} \right]$$
  
=  $\frac{1}{2} u(t_{i+1}, X_{i} + h\breve{b}_{i} - h^{1/2}\breve{\sigma}_{i}) + \frac{1}{2} u(t_{i+1}, X_{i} + h\breve{b}_{i} + h^{1/2}\breve{\sigma}_{i}) + h\breve{g}_{i}.$  (3.15)

Expanding the functions  $u(t_{i+1}, X_i + h\breve{b}_i \pm h^{1/2}\breve{\sigma}_i)$  at the point  $(t_i, X_i)$ , we get

$$u(t_{i+1}, X_i + h\breve{b}_i \pm h^{1/2}\breve{\sigma}_i) = u(t_i, X_i) + \frac{\partial u}{\partial t}h + (h\breve{b}_i \pm h^{1/2}\breve{\sigma}_i)\frac{\partial u}{\partial x} + \frac{\breve{\sigma}_i^2}{2}\frac{\partial^2 u}{\partial x^2}h \pm \breve{b}_i\breve{\sigma}_i\frac{\partial^2 u}{\partial x^2}h^{3/2} \pm \breve{\sigma}_i\frac{\partial^2 u}{\partial t\partial x}h^{3/2} \pm \frac{\breve{\sigma}_i^3}{6}\frac{\partial^3 u}{\partial x^3}h^{3/2} + O(h^2),$$
(3.16)

where the derivatives are calculated at the point  $(t_i, X_i)$ .

Here we have to assume for a while that the value  $u(t_{i+1}, x) + R(t_{i+1}, x)$  for  $x \in [\alpha, \beta]$  remains in the interval  $(u \circ, u^\circ)$  for a sufficiently small *h* (see conditions (ii)). Clearly,  $R(t_N, x) = 0$ , and below we prove recurrently that  $R(t_i, x)$  is sufficiently small under a sufficiently small *h*. Thereupon, thanks to (3.1), this assumption will be justified for such *h*.

Then due to assumptions (i) and (ii), we obtain

$$b_{i}(x) = b(t_{i}, x, \bar{u}(t_{i+1}, x)) = b(t_{i}, x, u(t_{i+1}, x) + R(t_{i+1}, x))$$
  
=  $b(t_{i}, x, u(t_{i+1}, x)) + \Delta b(t_{i+1}, x) = b(t_{i}, x, u(t_{i}, x)) + \Delta b(t_{i+1}, x) + O(h)$   
=  $b_{i}(x) + \Delta b_{i}(x) + O(h),$  (3.17)

where  $\Delta b_i(x) := \Delta b(t_{i+1}, x)$ ,

$$|\Delta b_i(x)| \leq K |R(t_{i+1}, x)|, |O(h)| \leq Kh.$$

Analogously

$$\bar{\sigma}_{i}^{2}(x) = \sigma_{i}^{2}(x) + \Delta \sigma_{i}^{2}(x) + O(h), \ \bar{g}_{i}(x) = g_{i}(x) + \Delta g_{i}(x) + O(h),$$
$$|\Delta \sigma_{i}^{2}(x)|, \ |\Delta g_{i}(x)| \leqslant K |R(t_{i+1}, x)|.$$
(3.18)

Substituting (3.16) in (3.15) and taking into account (3.17)–(3.18), we come to the relation

$$A_{i} = h\left(\frac{\partial u}{\partial t} + b_{i}\frac{\partial u}{\partial x} + \frac{\sigma_{i}^{2}}{2}\frac{\partial^{2}u}{\partial x^{2}} + g_{i}\right) + r_{i} + O(h^{2}),$$

where

$$|r_i| \leq Kh|R(t_{i+1}, X_i)|, |O(h^2)| \leq Ch^2,$$

the derivatives are calculated at the point  $(t_i, X_i)$ , and  $b_i, \sigma_i, g_i$  are calculated at  $(t_i, X_i, u(t_i, X_i))$ . Since u(t, x) is the solution of problem (2.1)–(2.3), this relation implies

$$A_i = r_i + \mathcal{O}(h^2).$$

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Therefore

$$R^{(1)}(t_k, x) = \sum_{i=k}^{N-1} E I_{\overline{Q} \setminus \partial \Gamma}(t_i, X_i) [r_i + O(h^2)].$$
(3.19)

Now consider  $R^{(2)}(t_k, x)$ . Let  $(t_i, X_i) \in \partial \Gamma$  be such that  $X_i$  is close to  $\alpha$ . Then according to (3.11), we obtain

$$B_{i} := E \left[ u(t_{i+1}, X_{i+1}) - u(t_{i}, X_{i}) + Z_{i+1} - Z_{i} / X_{i}, Z_{i} \right]$$
  
=  $u(t_{i+1}, X_{i} + \Delta X_{i}^{\alpha}) - u(t_{i}, X_{i}) - \psi_{1}(t_{i+1})(\Delta X_{i}^{\alpha} - h\breve{b}_{i}) + h\breve{g}_{i}$   
=  $u(t_{i+1}, X_{i} + \Delta X_{i}^{\alpha}) - u(t_{i}, X_{i}) - \frac{\partial u}{\partial x}(t_{i+1}, \alpha) \cdot (\Delta X_{i}^{\alpha} - h\breve{b}_{i}) + h\breve{g}_{i}.$  (3.20)

We evaluate this conditional expectation using the same arguments as in (3.15). Clearly

$$|X_i - \alpha| \leqslant C\sqrt{h}, \ |\Delta X_i^{\alpha}| \leqslant C\sqrt{h}.$$
(3.21)

Expanding the terms of (3.20) at the point  $(t_i, X_i)$  and taking into account assumptions (i), (ii), relations (3.17), (3.18), and (3.21), we obtain (see (3.9), (3.10)):

$$B_i = h\left(\frac{\partial u}{\partial t} + b_i \frac{\partial u}{\partial x} + \frac{\sigma_i^2}{2} \frac{\partial^2 u}{\partial x^2} + g_i\right) + \bar{r}_i + O(h^{3/2}),$$

where

$$|\bar{r}_i| \leqslant Kh |R(t_{i+1}, X_i)|,$$

the derivatives are calculated at the point  $(t_i, X_i)$ , and  $b_i, \sigma_i, g_i$  are calculated at  $(t_i, X_i, u(t_i, X_i))$ . Since u(t, x) is the solution of problem (2.1)–(2.3), this relation implies

$$B_i = \bar{r}_i + \mathcal{O}(h^{3/2}).$$

An analogous relation can be obtained for  $(t_i, X_i) \in \partial \Gamma$  with  $X_i$  being close to  $\beta$ . Therefore

$$R^{(2)}(t_k, x) = \sum_{i=k}^{N-1} E I_{\partial \Gamma}(t_i, X_i) [\bar{r}_i + O(h^{3/2})].$$
(3.22)

Substituting (3.19) and (3.22) in (3.13), we get

$$R(t_k, x) = \sum_{i=k}^{N-1} EI_{\overline{Q}\setminus\partial\Gamma}(t_i, X_i)[r_i + O(h^2)] + \sum_{i=k}^{N-1} EI_{\partial\Gamma}(t_i, X_i)[\bar{r}_i + O(h^{3/2})].$$
(3.23)

Let  $R_k := \max_{x \in [\alpha,\beta]} |R(t_k, x)|$ . Due to Lemma 3.2, we obtain from (3.23)

$$R_k \leqslant Kh \sum_{i=k}^{N-1} R_{i+1} + Ch.$$
 (3.24)

Introduce  $\varepsilon_k := Kh \sum_{i=k}^{N-1} R_{i+1} + Ch$ ,  $k = N - 1, \dots, 0$ . From (3.24)  $R_k \leq \varepsilon_k$  and consequently  $\varepsilon_k = KhR_{k+1} + \varepsilon_{k+1} \leq (1 + Kh)\varepsilon_{k+1}$ ,  $k = N - 2, \dots, 0$ . Then (since  $\varepsilon_{N-1} = Ch$ )

$$R_k \leq \varepsilon_k \leq C e^{K(T-t_0)} \cdot h, \ k = N, \dots, 0.$$

REMARK 3.1 Apparently, the conclusion of Theorem 3.1 is true under the boundary conditions (2.3). We have not succeeded in proving such a general theorem but we can prove it in the case of the linear boundary conditions

$$\frac{\partial u}{\partial x}(t,\alpha) = \varphi_1(t)u(t,\alpha) + \psi_1(t), \ \frac{\partial u}{\partial x}(t,\beta) = \varphi_2(t)u(t,\beta) + \psi_2(t), \ t_0 \leqslant t \leqslant T,$$
(3.25)

(the corresponding proof is rather long in comparison with the case of (3.12) and is not given here). Moreover, numerical experiments confirm the just mentioned conjecture (see Section 7.1).

It turns out that method (2.10) in the case (3.12) (and in the case (3.25) as well) is convergent with order  $O(h^{1/2})$ . As above, this fact is apparently true for the general case of boundary conditions.

Let us formulate the corresponding results. First we note that the method (2.10) generates a Markov chain  $(t_i, X_i)$  for which Lemma 3.2 takes place.

LEMMA 3.3 Under assumptions (i) and (ii), the one-step error  $\rho(t_k, x)$  of method (2.10) is estimated as

$$|\rho(t_k, x)| = |v(t_k, x) - u(t_k, x)| \leq Ch^2, \ x + hb_k \pm h^{1/2}\sigma_k \in [\alpha, \beta];$$

 $|\rho(t_k, x)| = |v(t_k, x) - u(t_k, x)| \leq Ch, \ x + hb_k - h^{1/2}\sigma_k < \alpha \text{ or } x + hb_k + h^{1/2}\sigma_k > \beta,$ 

where  $v(t_k, x)$  is defined by (2.9), C does not depend on h, k, x.

THEOREM 3.2 Under assumptions (i) and (ii), the method (2.10) for the Neumann problem (2.1)–(2.3), (3.12) is  $O(h^{1/2})$ , i.e.

$$|\bar{u}(t_k, x) - u(t_k, x)| \leqslant K h^{1/2}, \tag{3.26}$$

where K does not depend on h, k, x.

Proofs of Lemma 3.3 and Theorem 3.2 are similar to that of Lemma 3.1 and Theorem 3.1, and we do not give them here.

REMARK 3.2 The layer method (2.10) has the parameter q, which, in principle, may be any positive number. Naturally, the value of q affects the method accuracy: K of (3.26) depends on q. By an extended analysis of the one-step boundary error and of the mean number of steps of the corresponding Markov chain in the boundary layer  $\partial \Gamma$ , we get

$$K \leqslant C_1 \cdot \left( \frac{1}{q} \max_{(t,x) \in \overline{Q}} \left| \frac{\partial u}{\partial t} \right| + \frac{q}{2} \max_{(t,x) \in \overline{Q}} \left| \frac{\partial^2 u}{\partial x^2} \right| \right) + C_2,$$

where  $C_i$ , i = 1, 2, do not depend on h, k, x, and q.

Evidently, both large and small values of q are not appropriate. If we know estimates of derivatives of the solution for a considered problem, it is not difficult to indicate an appropriate q. But generally the choice of q requires special consideration.

Let  $b(t, x, u) \equiv 0$  and  $g(t, x, u) \equiv 0$ . In this case the one-step boundary error  $\rho(t_k, x)$  of method (2.10) near  $\alpha$  is evaluated as

$$\rho(t_k, x) = \frac{1}{2} \frac{\partial^2 u}{\partial x^2}(t_k, x) \cdot (q^2 h + 2(x - \alpha)qh^{1/2} - h\sigma_k^2) + \mathcal{O}(h^{3/2}), \ x - h^{1/2}\sigma_k < \alpha,$$

and analogously near  $\beta$ . Taking  $qh^{1/2} = \alpha - x + \sqrt{h\sigma_k^2 + (\alpha - x)^2}$ , we obtain  $\rho(t_k, x) = O(h^{3/2})$ . Substitution of such q (depending on k and x) in (2.10) gives us a method with convergence order O(h), which coincides with the method (2.7). Such an analysis also suggests that it is preferable to take  $q \approx \sigma$ .

#### 4. Numerical algorithms

To become numerical algorithms, the layer methods of Section 2 need a discretization in the variable *x*. Consider the equidistant space discretization with space step  $h_x$  (recall that the notation for time step is *h*):  $x_j = \alpha + jh_x$ , j = 0, 1, 2, ..., M,  $h_x = (\beta - \alpha)/M$ .

Using linear interpolation, we construct the following algorithm on the basis of method (2.7) (we denote it as  $\bar{u}(t_k, x)$  again, since this should not cause any confusion):

$$\begin{split} \bar{u}(t_{N}, x) &= \varphi(t_{N}, x), \ x \in [\alpha, \beta], \\ \bar{u}(t_{k}, x_{j}) &= \frac{1}{2}\bar{u}(t_{k+1}, x_{j} + h\bar{b}_{k,j} - h^{1/2}\bar{\sigma}_{k,j}) + \frac{1}{2}\bar{u}(t_{k+1}, x_{j} + h\bar{b}_{k,j} + h^{1/2}\bar{\sigma}_{k,j}) + h\bar{g}_{k,j}, \\ & \text{if } x_{j} + h\bar{b}_{k,j} \pm h^{1/2}\bar{\sigma}_{k,j} \in [\alpha, \beta]; \\ \bar{u}(t_{k}, x_{j}) &= \bar{u}(t_{k+1}, \alpha + \sqrt{h\bar{\sigma}_{k,j}^{2} + (\alpha - x_{j})^{2}}) \\ & -\psi_{1}(t_{k+1}, \bar{u}(t_{k+1}, \alpha)) \cdot (\alpha - x_{j} - h\bar{b}_{k,j} + \sqrt{h\bar{\sigma}_{k,j}^{2} + (\alpha - x_{j})^{2}}) + h\bar{g}_{k,j}, \\ & \text{if } x_{j} + h\bar{b}_{k,j} - h^{1/2}\bar{\sigma}_{k,j} < \alpha; \\ \bar{u}(t_{k}, x_{j}) &= \bar{u}(t_{k+1}, \beta - \sqrt{h\bar{\sigma}_{k,j}^{2} + (\beta - x_{j})^{2}}) \\ & -\psi_{2}(t_{k+1}, \bar{u}(t_{k+1}, \beta)) \cdot (\beta - x_{j} - h\bar{b}_{k,j} - \sqrt{h\bar{\sigma}_{k,j}^{2} + (\beta - x_{j})^{2}}) + h\bar{g}_{k,j}, \\ & \text{if } x_{j} + h\bar{b}_{k,j} + h^{1/2}\bar{\sigma}_{k,j} > \beta; \ j = 1, 2, \dots, M - 1, \end{split}$$

$$(4.1)$$

$$\bar{u}(t_k, x) = \frac{x_{j+1} - x}{h_x} \bar{u}(t_k, x_j) + \frac{x - x_j}{h_x} \bar{u}(t_k, x_{j+1}), \ x_j < x < x_{j+1},$$
  
$$j = 0, 1, 2, \dots, M - 1, \ k = N - 1, \dots, 1, 0,$$
 (4.2)

where  $\bar{b}_{k,j}$ ,  $\bar{\sigma}_{k,j}$ ,  $\bar{g}_{k,j}$  are the coefficients  $b, \sigma, g$  calculated at the point  $(t_k, x_j, \bar{u}(t_{k+1}, x_j))$ .

THEOREM 4.1 Consider the problem (2.1)–(2.3), (3.12). If the value of  $h_x$  is taken equal to  $\varkappa h$ ,  $\varkappa$  is a positive constant, then under assumptions (i) and (ii) the algorithm (4.1)–(4.2)

has the first order of convergence, i.e. the approximation  $\bar{u}(t_k, x)$  from formulae (4.1)–(4.2) satisfies the relation

$$|\bar{u}(t_k, x) - u(t_k, x)| \leq Kh,$$

where K does not depend on x, h, k.

*Proof.* In connection with the algorithm (4.1)–(4.2), we introduce the random sequence  $X_i, Z_i, i = k, ..., N$ . We put  $X_k = x_j, Z_k = 0$  (to avoid confusion, we note that the index k of  $X_k, Z_k$  means that  $X_k, Z_k$  belong to the kth time layer, while the index j of  $x_j$  corresponds to the space discretization introduced at the beginning of this section) and then

$$X_{i+1}^{\pm} := X_i + h\breve{b}_i \pm h^{1/2}\breve{\sigma}_i, \ i = k, \dots, N-1.$$
(4.3)

For i = k, ..., N - 2:

$$\begin{split} \text{if } X_{i+1}^{\pm} \in [\alpha, \beta], \text{ then } P(X_{i+1} = x_l) &= \frac{1}{2} \frac{x_{l+1} - X_{i+1}^-}{h_x}, \ P(X_{i+1} = x_{l+1}) = \frac{1}{2} \frac{X_{i+1}^- - x_l}{h_x}, \\ P(X_{i+1} = x_m) &= \frac{1}{2} \frac{x_{m+1} - X_{i+1}^+}{h_x}, \ P(X_{i+1} = x_{m+1}) = \frac{1}{2} \frac{X_{i+1}^+ - x_m}{h_x}, \ Z_{i+1} = Z_i + h\check{g}_i, \\ \text{where } x_l, \ x_{l+1}, \ x_m, \ x_{m+1} \text{ are such that } x_l \in X_{i+1}^- < x_{l+1}, \ x_m < X_{i+1}^+ \in x_{m+1}; \\ \text{ if } X_{i+1}^- < \alpha, \ \text{then} \\ P(X_{i+1} = x_m) &= \frac{x_{m+1} - (X_i + \Delta X_i^{\alpha})}{h_x}, \ P(X_{i+1} = x_{m+1}) = \frac{(X_i + \Delta X_i^{\alpha}) - x_m}{h_x}, \\ Z_{i+1} = Z_i + h\check{g}_i - \psi_1(t_{i+1}) \cdot (\Delta X_i^{\alpha} - h\check{b}_i), \\ \text{where } \Delta X_i^{\alpha} &= (\alpha - X_i) + \sqrt{h\check{\sigma}_i^2 + (\alpha - X_i)^2} \text{ and } x_m, \ x_{m+1} \text{ are such that} \\ x_m < X_i + \Delta X_i^{\alpha} \leqslant x_{m+1}; \\ \text{ if } X_{i+1}^+ > \beta, \ \text{then} \\ P(X_{i+1} = x_l) &= \frac{x_{l+1} - (X_i + \Delta X_i^{\beta})}{h_x}, \ P(X_{i+1} = x_{l+1}) = \frac{(X_i + \Delta X_i^{\beta}) - x_l}{h_x}, \\ Z_{i+1} = Z_i + h\check{g}_i - \psi_2(t_{i+1}) \cdot (\Delta X_i^{\beta} - h\check{b}_i), \\ \text{where } \Delta X_i^{\beta} &= (\beta - X_i) - \sqrt{h\check{\sigma}_i^2 + (\beta - X_i)^2} \text{ and } x_l, \ x_{l+1} \text{ are such that} \\ x_l &\in X_i + \Delta X_i^{\beta} < x_{l+1}. \end{split}$$

For i = N - 1:

if 
$$X_N^{\pm} \in [\alpha, \beta]$$
, then  $P(X_N = X_N^-) = P(X_N = X_N^+) = \frac{1}{2}$ ,  $Z_N = Z_{N-1} + h\check{g}_{N-1}$ ;  
if  $X_N^- < \alpha$ , then (4.4)

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$$\begin{split} X_N &= X_{N-1} + \Delta X_{N-1}^{\alpha}, \ Z_N = Z_{N-1} + h \check{g}_{N-1} - \psi_1(t_N) \cdot (\Delta X_{N-1}^{\alpha} - h \check{b}_{N-1}), \\ & \text{where } \Delta X_{N-1}^{\alpha} = (\alpha - X_{N-1}) + \sqrt{h \check{\sigma}_{N-1}^2 + (\alpha - X_{N-1})^2}; \\ & \text{if } X_N^+ > \beta, \text{ then} \\ & X_N = X_{N-1} + \Delta X_{N-1}^{\beta}, \ Z_N = Z_{N-1} + h \check{g}_{N-1} - \psi_2(t_N) \cdot (\Delta X_{N-1}^{\beta} - h \check{b}_{N-1}), \\ & \text{where } \Delta X_{N-1}^{\beta} = (\beta - X_{N-1}) - \sqrt{h \check{\sigma}_{N-1}^2 + (\beta - X_{N-1})^2}. \end{split}$$

Here  $\check{b}_i = \bar{b}_i(X_i) = b(t_i, X_i, \bar{u}(t_{i+1}, X_i)), \ \check{\sigma}_i = \bar{\sigma}_i(X_i) = \sigma(t_i, X_i, \bar{u}(t_{i+1}, X_i)), \ \text{and} \ \check{g}_i = \bar{g}_i(X_i) = g(t_i, X_i, \bar{u}(t_{i+1}, X_i)).$ 

It is clear that

$$\bar{u}(t_k, x_j) = E[\bar{u}(t_N, X_N) + Z_N] = E[\varphi(t_N, X_N) + Z_N] = E[u(t_N, X_N) + Z_N].$$

Introduce the notation

$$R(t_k, x) := \bar{u}(t_k, x) - u(t_k, x), \ R_k := \max_{x \in [\alpha, \beta]} |R(t_k, x)|.$$

Using arguments similar to those which led us to (3.23) and taking into account that the error of linear interpolation is  $O(h_x^2)$ , we get

$$R(t_k, x_j) = \sum_{i=k}^{N-1} E I_{\overline{Q} \setminus \partial \Gamma}(t_i, X_i) [r_i + O(h^2) + O(h_x^2)] + \sum_{i=k}^{N-1} E I_{\partial \Gamma}(t_i, X_i) [\bar{r}_i + O(h^{3/2}) + O(h_x^2)],$$
(4.5)

where

$$|r_i|, |\bar{r}_i| \leq Kh|R(t_{i+1}, X_i)|.$$

A lemma similar to Lemma 3.2 can be proved for the Markov chain  $(t_i, X_i)$  defined by (4.3). Then, we obtain from (4.5) for  $h_x = \varkappa h$ :

$$|R(t_k, x_j)| \leq Kh \sum_{i=k}^{N-1} R_{i+1} + Ch.$$
(4.6)

We have

$$u(t_k, x) = \frac{x_{j+1} - x}{h_x} u(t_k, x_j) + \frac{x - x_j}{h_x} u(t_k, x_{j+1}) + O(h_x^2), \ x_j \le x \le x_{j+1}.$$
 (4.7)

From (4.7) and (4.2),

$$R(t_k, x) = \frac{x_{j+1} - x}{\varkappa h} R(t_k, x_j) + \frac{x - x_j}{\varkappa h} R(t_k, x_{j+1}) + O(h^2),$$

whence due to (4.6)

$$|R(t_k, x)| \leq Kh \sum_{i=k}^{N-1} R_{i+1} + Ch.$$

Consequently we get (3.24).

REMARK 4.1 We pay attention to the fact that the factor  $\varkappa$  in Theorem 4.1 is arbitrary. To choose  $h_{\chi}$ , we do not need any stability criteria in comparison to finite-difference schemes, on which the Lax–Richtmayer equivalence theorem imposes a requirement on relation between the time step  $\Delta t$  and the space step  $\Delta x$  (see Milstein (1997) for a detailed discussion). At the same time, accuracy of the algorithm (4.1)–(4.2) depends on  $\varkappa$ . In practice, a choice of  $\varkappa$  is connected with interpolation properties of the solution.

REMARK 4.2 An exploitation of cubic interpolation allows us to take the space step  $h_x = \varkappa \sqrt{h}$  (in contrast to  $h_x = \varkappa h$  for the linear interpolation) and, thus, to reduce the volume of computations. Unfortunately, we have not succeeded in proving a convergence theorem for algorithms with cubic interpolation. In Section 7 we test such algorithms which give fairly good results. See also some theoretical explanations and numerical tests in Milstein (1997) and Milstein & Tretyakov (2000a, 2001).

On the basis of linear interpolation and the layer method (2.10), we get the following algorithm:

$$\bar{u}(t_{N}, x) = \varphi(t_{N}, x), \ x \in [\alpha, \beta],$$

$$\bar{u}(t_{k}, x_{j}) = \frac{1}{2}\bar{u}(t_{k+1}, x_{j} + h\bar{b}_{k,j} - h^{1/2}\bar{\sigma}_{k,j}) + \frac{1}{2}\bar{u}(t_{k+1}, x_{j} + h\bar{b}_{k,j} + h^{1/2}\bar{\sigma}_{k,j}) + h\bar{g}_{k,j},$$

$$\text{if } x_{j} + h\bar{b}_{k,j} \pm h^{1/2}\bar{\sigma}_{k,j} \in [\alpha, \beta];$$

$$\bar{u}(t_{k}, x_{j}) = \bar{u}(t_{k+1}, x_{j} + q\sqrt{h}) - \psi_{1}(t_{k+1}, \bar{u}(t_{k+1}, \alpha)) \cdot qh^{1/2},$$

$$\text{if } x_{j} + h\bar{b}_{k,j} - h^{1/2}\bar{\sigma}_{k,j} < \alpha;$$

$$\bar{u}(t_{k}, x_{j}) = \bar{u}(t_{k+1}, x_{j} - q\sqrt{h}) + \psi_{2}(t_{k+1}, \bar{u}(t_{k+1}, \beta)) \cdot qh^{1/2},$$

$$\text{if } x_{j} + h\bar{b}_{k,j} + h^{1/2}\bar{\sigma}_{k,j} > \beta; \ j = 1, 2, \dots, M-1,$$

$$(4.8)$$

$$\bar{u}(t_k, x) = \frac{x_{j+1} - x}{h_x} \bar{u}(t_k, x_j) + \frac{x - x_j}{h_x} \bar{u}(t_k, x_{j+1}), \ x_j < x < x_{j+1},$$
  
$$j = 0, 1, 2, \dots, M - 1, \ k = N - 1, \dots, 1, 0,$$
 (4.9)

where  $\bar{b}_{k,j}$ ,  $\bar{\sigma}_{k,j}$ ,  $\bar{g}_{k,j}$  are the coefficients  $b, \sigma, g$  calculated at the point  $(t_k, x_j, \bar{u}(t_{k+1}, x_j))$ . THEOREM 4.2 Consider the problem (2.1)–(2.3), (3.12). If the value of  $h_x$  is taken equal to  $\varkappa h^{3/4}$ ,  $\varkappa$  is a positive constant, then under assumptions (i) and (ii) the algorithm (4.8)–(4.9) has order of convergence  $O(\sqrt{h})$ , i.e. the approximation  $\bar{u}(t_k, x)$  from formulae (4.8)–(4.9) satisfies the relation

$$|\bar{u}(t_k, x) - u(t_k, x)| \leq K\sqrt{h},$$

where K does not depend on x, h, k.

This theorem is proved by the same arguments as Theorem 4.1.

# 5. Extension to the multi-dimensional Neumann problem

It is not difficult to generalize the layer methods given above to an arbitrary d. For instance, let us extend the method (2.10) to the case of d = 2. Recall that  $\sigma$  is a 2 × 2-matrix satisfying the relation  $\sigma\sigma^{\top} = a$ .

Introduce the notation  $_{i}X_{k+1} := (_{i}X_{k+1}^{1}, _{i}X_{k+1}^{2}),$ 

$${}_{i}X_{k+1}^{1} = x^{1} + \bar{b}_{k}^{1}h + \bar{\sigma}_{k}^{11}\sqrt{h} \cdot {}_{i}\xi^{1} + \bar{\sigma}_{k}^{12}\sqrt{h} \cdot {}_{i}\xi^{2},$$
  

$${}_{i}X_{k+1}^{2} = x^{2} + \bar{b}_{k}^{2}h + \bar{\sigma}_{k}^{21}\sqrt{h} \cdot {}_{i}\xi^{1} + \bar{\sigma}_{k}^{22}\sqrt{h} \cdot {}_{i}\xi^{2},$$
  

$$i = 1, 2, 3, 4, \ x = (x^{1}, x^{2}) \in \overline{G} \subset \mathbb{R}^{2},$$

where  $_{1}\xi = (-1, -1), _{2}\xi = (-1, 1), _{3}\xi = -_{1}\xi, _{4}\xi = -_{2}\xi$  and  $\bar{b}_{k} = (\bar{b}_{k}^{1}, \bar{b}_{k}^{2}), \bar{\sigma}_{k} = \{\bar{\sigma}_{k}^{jl}\}$ are the coefficients b(t, x, u),  $\sigma(t, x, u)$  calculated at the point  $(t_k, x, \overline{u}(t_{k+1}, x))$ .

If the point  $x = (x^1, x^2) \in G$  is sufficiently far from the boundary  $\partial G$  (more precisely, if the points  $_{i}X_{k+1}$ , i = 1, 2, 3, 4, belong to  $\overline{G}$ ), the layer method has the form (see Milstein (1997), Milstein & Tretyakov (2001)):

$$\bar{u}(t_k, x^1, x^2) = \sum_{i=1}^4 \frac{1}{4} \bar{u}(t_{k+1}, \, _i X^1_{k+1}, \, _i X^2_{k+1}) + \bar{g}_k \cdot h, \tag{5.1}$$

where  $\bar{g}_k$  is the coefficient g(t, x, u) calculated at the point  $(t_k, x, \bar{u}(t_{k+1}, x))$ . If the point  $x = (x^1, x^2) \in \overline{G}$  is close or belongs to the boundary  $\partial G$ , then some of the points  $_{i}X_{k+1} = (_{i}X_{k+1}^{1}, _{i}X_{k+1}^{2}), i = 1, 2, 3, 4$ , may be outside of the domain  $\overline{G}$ . In this case let us consider the projection  $\bar{x}$  of the point x on  $\partial G$ . Let  $\nu = (\nu^1, \nu^2)$  be the unit vector of the internal normal at the point  $\bar{x}$ . Clearly, if  $x \neq \bar{x}$ ,  $\nu = (x - \bar{x})/|x - \bar{x}|$ . Then we put

$$\bar{u}(t_k, x^1, x^2) = \bar{u}(t_{k+1}, x + qh^{1/2}\nu) - \psi(t_{k+1}, \bar{x}, \bar{u}(t_{k+1}, \bar{x})) \cdot qh^{1/2}.$$
 (5.2)

Thus, we obtain the method (5.1)–(5.2): the rule (5.1) is to be for points  $x = (x^1, x^2) \in$ G such that all the corresponding points  $_{i}X = (_{i}X^{1}, _{i}X^{2}), i = 1, 2, 3, 4$ , belong to  $\overline{G}$ , and the rule (5.2) is to be otherwise. The error of the one-step approximation corresponding to (5.1) is  $O(h^2)$  and that corresponding to (5.2) is O(h). If the function  $\psi$  does not depend on u, we can prove that the layer method (5.1)–(5.2) has the global error estimated by  $O(h^{1/2})$ . These assertions can be checked directly without requiring new ideas than those in Section 3.

To construct the corresponding numerical algorithms, we use linear interpolation as in the previous section. If the domain G is a rectangle  $\Pi$  with corners  $(x_0^1, x_0^2), (x_0^1, x_{M_2}^2), (x_0^1, x_{M_2}^2)$  $(x_{M_1}^1, x_0^2), (x_{M_1}^1, x_{M_2}^2)$ , we introduce the equidistant space discretization:

$$\Delta_{M_1,M_2} := \{ (x_j^1, x_l^2) : x_j^1 = x_0^1 + jh_{x^1}, x_l^2 = x_0^2 + lh_{x^2}, j = 0, \dots, M_1, l = 0, \dots, M_2 \}$$
$$h_{x^1} = \frac{x_{M_1}^1 - x_0^1}{M_1}, h_{x^2} = \frac{x_{M_2}^2 - x_0^2}{M_2}.$$

The values of  $\bar{u}(t_k, x_i^1, x_i^2)$  at the nodes of  $\Delta_{M_1, M_2}$  are found in accordance with (5.1)– (5.2). Let  $x_j^1 < x^1 < x_{j+1}^1$ ,  $x_l^2 < x^2 < x_{l+1}^2$ . Then the value of  $\bar{u}(t_k, x^1, x^2)$  is evaluated

$$\bar{u}(t_k, x^1, x^2) = \frac{x_{j+1}^1 - x^1}{h_{x^1}} \cdot \frac{x_{l+1}^2 - x^2}{h_{x^2}} \bar{u}(t_k, x_j^1, x_l^2) + \frac{x_{j+1}^1 - x^1}{h_{x^1}} \cdot \frac{x^2 - x_l^2}{h_{x^2}} \bar{u}(t_k, x_j^1, x_{l+1}^2) + \frac{x^1 - x_j^1}{h_{x^1}} \cdot \frac{x^2 - x_l^2}{h_{x^2}} \bar{u}(t_k, x_{j+1}^1, x_{l+1}^2) + \frac{x^1 - x_j^1}{h_{x^1}} \cdot \frac{x^2 - x_l^2}{h_{x^2}} \bar{u}(t_k, x_{j+1}^1, x_{l+1}^2).$$
(5.3)

If the function  $\psi$  does not depend on u, we can prove that taking  $h_{x^i} = x^i h^{3/4}$ ,  $i = 1, 2, x^1, x^2 > 0$ , the error of this algorithm is estimated as  $O(h^{1/2})$ .

The case of an arbitrary domain G requires a special consideration. For instance, for a sufficiently wide class of domains G, it is possible to find one-to-one mapping of G onto a domain G' with a rectangular grid (see e.g. Fletcher (1991) and references therein). Then we can use the above given algorithm in G' and map the results onto G.

REMARK 5.1 Combining methods from Milstein & Tretyakov (2001) and from this paper, we can solve mixed boundary value problems, i.e. when we have the Dirichlet condition on a part of the boundary  $\partial G$  and the Neumann condition on the rest of  $\partial G$ .

## 6. Some other layer methods

In this section two additional methods in the case of d = 1 are given.

Using the concept of fictitious knots, we obtain the following method (see details in Milstein & Tretyakov (2000b)):

$$\begin{split} \bar{u}(t_N, x) &= \varphi(x), \ x \in [\alpha, \beta], \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \\ &\text{if } x + h\bar{b}_k \pm h^{1/2}\bar{\sigma}_k \in [\alpha, \beta], \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, 2\alpha - x - h\bar{b}_k + h^{1/2}\bar{\sigma}_k) \\ &-\psi_1(t_{k+1}, \bar{u}(t_{k+1}, \alpha)) \cdot (\alpha - x - h\bar{b}_k + h^{1/2}\bar{\sigma}_k) \\ &+ \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \ \text{if } x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k < \alpha, \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2}\bar{u}(t_{k+1}, 2\beta - x - h\bar{b}_k - h^{1/2}\bar{\sigma}_k) \\ &+ \psi_2(t_{k+1}, \bar{u}(t_{k+1}, \beta)) \cdot (x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k - \beta) + h\bar{g}_k, \\ &\text{if } x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k > \beta; \\ &k = N - 1, \dots, 1, 0, \end{split}$$
(6.1)

where  $\bar{b}_k$ ,  $\bar{\sigma}_k$ ,  $\bar{g}_k$  are the coefficients b,  $\sigma$ , g calculated at the point  $(t_k, x, \bar{u}(t_{k+1}, x))$ .

The method (6.1) is an explicit layer method for solving the Neumann problem (2.1)–(2.3). We prove that its one-step error near the boundary is  $O(h^{3/2})$  and for internal points is  $O(h^2)$ . Apparently, this method has order of convergence O(h).

The method (6.1) is more complicated than the method (2.7). At the same time it demonstrates more accurate results than (2.7) in our numerical tests (see Section 7.1).

The method (2.10) is an extension of the method of  $O(h^{1/2})$  from Milstein (1996) to the nonlinear case. In Costantini *et al.* (1998) another method of  $O(h^{1/2})$  is proposed. Its

extension to the nonlinear Neumann problem (2.1)-(2.3) has the form

$$\begin{split} \bar{u}(t_N, x) &= \varphi(t_N, x), \ x \in [\alpha, \beta], \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \\ &\text{if } x + h\bar{b}_k \pm h^{1/2}\bar{\sigma}_k \in [\alpha, \beta]; \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, \alpha) + \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k) \\ -\frac{1}{2}\psi_1(t_{k+1}, \bar{u}(t_{k+1}, \alpha))(\alpha - x - h\bar{b}_k + h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \ \text{if } x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k < \alpha; \\ \bar{u}(t_k, x) &= \frac{1}{2}\bar{u}(t_{k+1}, x + h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + \frac{1}{2}\bar{u}(t_{k+1}, \beta) \\ -\frac{1}{2}\psi_2(t_{k+1}, \bar{u}(t_{k+1}, \beta))(\beta - x - h\bar{b}_k - h^{1/2}\bar{\sigma}_k) + h\bar{g}_k, \ \text{if } x + h\bar{b}_k + h^{1/2}\bar{\sigma}_k > \beta; \\ k = N - 1, \dots, 1, 0, \end{split}$$
(6.2)

where  $\bar{b}_k = \bar{b}_k(x) = b(t_k, x, \bar{u}(t_{k+1}, x)), \ \bar{\sigma}_k = \bar{\sigma}_k(x) = \sigma(t_k, x, \bar{u}(t_{k+1}, x)), \ \bar{g}_k = \bar{g}_k(x) = g(t_k, x, \bar{u}(t_{k+1}, x)).$ 

We prove that the one-step error of this method near the boundary is O(h) and for internal points is  $O(h^2)$ . Apparently, this layer method has order of convergence  $O(h^{1/2})$ . It is more complicated near the boundary than (2.10). At the same time the method (6.2) demonstrates more accurate results than (2.10) in our numerical tests (see Section 7.1).

Algorithms based on linear interpolation and layer methods of this section can be written down as in Section 4 for the methods from Section 2.

## 7. Numerical tests

# 7.1 Tests of various layer methods

Consider the Neumann problem for the one-dimensional Burgers equation:

$$\frac{\partial u}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}, \quad t > 0, \ x \in (-4, 4),$$
(7.1)

$$u(0, x) = -\frac{\sigma^2 \sinh x}{\cosh x + A}, \ x \in [-4, 4],$$
(7.2)

$$\frac{\partial u}{\partial x}(t, \pm 4) = -\sigma^2 \frac{1 + A \exp(-\sigma^2 t/2) \cosh 4}{[\cosh 4 + A \exp(-\sigma^2 t/2)]^2}, \ t \ge 0.$$
(7.3)

Here A is a positive constant.

The exact solution to this problem has the form (see Benton & Platzman (1972))

$$u(t, x) = -\frac{\sigma^2 \sinh x}{\cosh x + A \exp(-\sigma^2 t/2)}.$$

In the tests we use cubic interpolation (see Remark 4.2)

$$\bar{u}(t_k, x) = \sum_{i=0}^{3} \Phi_{j,i}(x)\bar{u}(t_k, x_{j+i}), \quad x_j < x < x_{j+3},$$
$$\Phi_{j,i}(x) = \prod_{m=0, m \neq i}^{3} \frac{x - x_{j+m}}{x_{j+i} - x_{j+m}}.$$
(7.4)

h	algorithms					
	(4.1)–(4.2)	(4.1), (7.4)	(6.1), (7.4)	(4.8), (7.4)	(6.2), (7.4)	
0.16	$5.216 \cdot 10^{-1}$	$7.434 \cdot 10^{-1}$	$5.967 \cdot 10^{-2}$	> 1	$7.333 \cdot 10^{-1}$	
	$8 \cdot 509 \cdot 10^{-2}$	$1.177 \cdot 10^{-1}$	$1.380 \cdot 10^{-2}$	$3\cdot 328\cdot 10^{-1}$	$1.098 \cdot 10^{-1}$	
0.01	$3 \cdot 170 \cdot 10^{-2}$	$1.888 \cdot 10^{-2}$	$3.867 \cdot 10^{-3}$	$3.722 \cdot 10^{-1}$	$1.346 \cdot 10^{-1}$	
	$5.748 \cdot 10^{-3}$	$3.737 \cdot 10^{-3}$	$1 \cdot 224 \cdot 10^{-3}$	$6 \cdot 161 \cdot 10^{-2}$	$2{\cdot}192\cdot10^{-2}$	
0.001	$4.479 \cdot 10^{-3}$	$3.835 \cdot 10^{-3}$	$7 \cdot 124 \cdot 10^{-4}$	$1.653 \cdot 10^{-1}$	$4{\cdot}909\cdot10^{-2}$	
	$^{\circ}8.149 \cdot 10^{-4}$	$7.444 \cdot 10^{-4}$	$2 \cdot 127 \cdot 10^{-4}$	$2{\cdot}750\cdot10^{-2}$	$8 \cdot 172 \cdot 10^{-3}$	
0.000	$12.387 \cdot 10^{-4}$	$2 \cdot 711 \cdot 10^{-4}$	$4{\cdot}639\cdot10^{-5}$	$4{\cdot}378\cdot10^{-2}$	$1 \cdot 168 \cdot 10^{-2}$	
	$4.479 \cdot 10^{-5}$	$5 \cdot 213 \cdot 10^{-5}$	$1{\cdot}357\cdot10^{-5}$	$7{\cdot}307\cdot10^{-3}$	$1.968 \cdot 10^{-3}$	

TABLE 1 Dependence of the errors  $err^{c}(t)$  (bottom position) and  $err^{l}(t)$  (top position) in h under t = 2,  $\sigma = 1.5$ , and A = 2.

Here we test the following five algorithms: (i) the algorithm (4.1)–(4.2), (ii) the algorithm based on layer method (2.7) and cubic interpolation (7.4), (iii) the algorithm based on layer method (6.1) and cubic interpolation (7.4), (iv) the algorithm based on layer method (2.10) and cubic interpolation (7.4), and (v) the algorithm based on layer method (6.2) and cubic interpolation (7.4). We take the space step  $h_x = h$  for linear interpolation and  $h_x = \sqrt{h}$  for cubic interpolation. The parameter q of algorithm (4.8), (7.4) is taken equal to 1.

Table 1 and Fig. 1 give numerical results obtained by these algorithms. In the table the errors of the approximate solutions  $\bar{u}$  are presented in the discrete Chebyshev norm (bottom position) and in  $l^1$ -norm (top position):

$$\operatorname{err}^{c}(t) = \max_{x_{i}} |\bar{u}(t, x_{i}) - u(t, x_{i})|,$$
  
$$\operatorname{err}^{l}(t) = \sum_{i} |\bar{u}(t, x_{i}) - u(t, x_{i})| \cdot h_{x}.$$
 (7.5)

In the experiments, the algorithm (4.8), (7.4) and the algorithm (6.2), (7.4) converge as  $O(h^{1/2})$ , the other algorithms converge as O(h). We note that the algorithm (6.2), (7.4) gives more accurate results than the algorithm (4.8), (7.4), and the algorithm (6.1), (7.4) is more accurate than the algorithms (4.1). The algorithms (4.1)–(4.2) and (4.1), (7.4) demonstrate almost the same accuracy. But the algorithm (4.1)–(4.2) (as well as other algorithms based on linear interpolation) requires both larger volume of computations per time layer and larger amount of memory than the algorithm (4.1), (7.4) based on cubic interpolation (see also Remark 4.2 in Section 4 and numerical tests in Milstein & Tretyakov (2001)).

Further, the boundary condition (7.3) can be rewritten in the form

$$\frac{\partial u}{\partial x}(t,\pm 4) = u(t,\pm 4) \left(\frac{1}{\sigma^2} u(t,\pm 4) - 1\right) - \frac{\sigma^2 \exp(\pm 4)}{\cosh 4 + A \exp(-\sigma^2 t/2)}, \ t \ge 0.$$
(7.6)

In order to provide an experimental verification of the conjecture from Remark 3.1 we apply the algorithm (4.1), (7.4) to (7.1) with the initial condition (7.2) and the nonlinear boundary condition (7.6). Taking the same values of parameters as in Table 1, we obtain,



FIG. 1. Solution of problem (7.1)–(7.3). Here h = 0.16, other parameters are as in Table 1.

in particular, that for h = 0.01 the error  $\operatorname{err}^{c}(2) = 1.103 \times 10^{-3}$  and for h = 0.0001 the error  $\operatorname{err}^{c}(2) = 1.138 \times 10^{-5}$  that experimentally confirms the conjecture.

# 7.2 A comparison analysis of layer methods and finite-difference schemes

Here the test problem is the Burgers equation

$$\frac{\partial u}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x}, \quad t > 0, \ x \in (-2, 8),$$
(7.7)

with the following initial and boundary conditions:

$$u(0, x) = \varphi(x) := \begin{cases} a, & x \in [-2, 0), \\ (a+b)/2, & x = 0, \\ b, & x \in (0, 8], \end{cases}$$
(7.8)

$$\frac{\partial u}{\partial x}(t,x) = \psi(t,x), \ t > 0, \ x \in \{-2,8\},$$
(7.9)

where

$$\psi(t,x) = -\frac{(a-b)^2 J_1(t,x) J_2(t,x)}{\sigma^2 \cdot (J_1(t,x) + J_2(t,x))^2} + \sqrt{\frac{2}{\pi\sigma^2 t}} \exp\left(\frac{-x^2}{2\sigma^2 t}\right) \frac{b-a}{J_1(t,x) + J_2(t,x)}$$

TABLE 2 Comparison analysis. Dependence of the errors  $err^{c}(t)$  (bottom position) and  $err^{l}(t)$  (top position) in h under t = 0.6,  $\sigma = 0.4$ , a = 11, and b = 9.

h	0.01	0.0016	0.0004	0.0001
algorithm	$4.859 \times 10^{-1}$	$1.031 \times 10^{-1}$	$2.659 \times 10^{-2}$	$6.792 \times 10^{-3}$
(4.1), (7.4)	1.208	$3.425 \times 10^{-1}$	$8.980 \times 10^{-2}$	$2{\cdot}308\times10^{-2}$
		2.531	$5.057 \times 10^{-2}$	$1.234 \times 10^{-2}$
scheme (7.10)	overflow	6.375	$1.261 \times 10^{-1}$	$2.766 \times 10^{-2}$
		oscillations		

and

$$J_1(t, x) = \exp\left(\frac{a(at-2x)}{2\sigma^2}\right) \operatorname{erfc}\left(\frac{x-at}{\sqrt{2\sigma^2 t}}\right),$$
$$J_2(t, x) = \exp\left(\frac{b(bt-2x)}{2\sigma^2}\right) \operatorname{erfc}\left(\frac{bt-x}{\sqrt{2\sigma^2 t}}\right).$$

The exact solution of this problem is

$$u(t,x) = \frac{aJ_1(t,x) + bJ_2(t,x)}{J_1(t,x) + J_2(t,x)}.$$

We compare the algorithm (4.1), (7.4) with the method of differences forward in time and central differences in space applied to the divergent form of the Burgers equation. This finite-difference scheme in application to the problem (7.7)–(7.9) is written as

$$\bar{u}(0,x) = \varphi(x), \ x \in [-2,8],$$

$$\bar{u}(t_{k+1},x_{-1}) = \bar{u}(t_{k+1},x_1) - 2\Delta x \cdot \psi(t_{k+1},x_0),$$

$$\bar{u}(t_{k+1},x_{M+1}) = \bar{u}(t_{k+1},x_{M-1}) + 2\Delta x \cdot \psi(t_{k+1},x_M),$$

$$\bar{u}(t_{k+1},x_j) = \bar{u}(t_k,x_j) - \frac{\Delta t}{4\Delta x}(\bar{u}^2(t_k,x_{j+1}) - \bar{u}^2(t_k,x_{j-1}))$$

$$+ \frac{\sigma^2}{2}\frac{\Delta t}{\Delta x^2}(\bar{u}(t_k,x_{j+1}) - 2\bar{u}(t_k,x_j) + \bar{u}(t_k,x_{j-1})),$$

$$j = 0, \dots, M, \ k = 0, \dots, N - 1,$$
(7.10)

where the step of time discretization  $\Delta t := T/N$  and  $t_k = k \cdot \Delta t$  and the step of space discretization  $\Delta x := 10/M$  and  $x_j = -2 + j \cdot \Delta x$ .

The explicit scheme (7.10) is of  $O(\Delta t, \Delta x^2)$ . It is used for simulation of the Burgers equation in Anderson *et al.* (1984) and Fletcher (1991).

In the experiments we take the space step  $h_x = \sqrt{h}$  for the algorithm (4.1), (7.4) and the space step  $\Delta x = \sqrt{\Delta t}$  for the finite-difference scheme (7.10) with the relationship  $\Delta t = h$ .

Table 2 presents the errors in the discrete Chebyshev norm (bottom position in the table) and in  $l^1$ -norm (top position) (see (7.5)). The comment 'overflow' indicates that overflow



FIG. 2. Solution of problem (7.7)–(7.9). Solid curve, exact solution; dotted curve, the algorithm (4.1); (7.4), dashed curve, the scheme (7.10). Here h = 0.0016, other parameters are as in Table 2.

error occurs during simulation. The comment 'oscillations' means that the numerical solution has oscillations (see Fig. 2). We see that the algorithm (4.1), (7.4) demonstrates a more stable behaviour than the finite-difference scheme (7.10). In the test problem (7.7)–(7.9) large values of *a*, *b* lead, in particular, to large advection in a neighbourhood of the front. These experiments confirm that the layer methods allow us to avoid difficulties stemming from strong advection (see also comparison analysis in Milstein & Tretyakov (2001)). We note that the algorithms based on layer methods require more CPU time than finite-difference schemes. For example, in the case of parameters as in Table 2 to solve (7.7)–(7.9) by the algorithm (4.1), (7.4) with h = 0.0004 we need  $\approx 5$  s while the scheme (7.10) requires  $\approx 2.8$  s. But the algorithm (4.1), (7.4) gives us quite appropriate results with the greater step h = 0.0016 (see Table 2 and Fig. 2) and in this case it requires  $\approx 0.7$  s. Simulations were made on a PC with Intel Pentium 233 MHz processor using Borland C compiler. A more extensive comparison analysis requires a separate consideration.

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