Numerical Solution of the Heat Equation in Unbounded Domains Using Quasi-uniform Grids

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Abstract. Numerical solutions of the heat equation on the semi-infinite interval in one dimension and on a strip in two dimensions with nonlinear boundary conditions are investigated. At the space discretization with respect to the variable on the semi-infinite interval, we use quasi-uniform mesh with finite number of intervals. Convergence results are formulated. Numerical experiments demonstrate the efficiency of the approximations. The results are compared with those, obtained by the well known method of artificial boundary conditions.

1 Introduction

Differential problems on unbounded domains require specific techniques for their numerical treatment. When solving numerically a problem formulated on an unbounded domain, one typically truncates this domain, which necessitate setting the artificial boundary conditions (ABCs) at the newly formed external boundary. This method is often used in problems of acoustic, electro-dynamics, solid and fluid mechanics [1,10,15,16]. For almost any problem formulated on an unbounded domain, there are many different ways of classing its counterpart. In other words, the choice of the ABCs is never unique. But, very often the construction of ABCs is not easy [9,11,15,16]. Also, the minimal necessary requirement of ABCs is to ensure the solvability of the truncated problem, which leads to additional computational work. Therefore it is reasonable to be developed another methods.

In this paper we derive second order approximations (with respect to space variables), using quasi-uniform meshes (QUMs) for 1D and 2D problems with dynamical or Neumann nonlinear boundary conditions on the bounded part of domain boundary. The algorithm, we develop is effective also for blow-up solutions, because it uses decreasing time step, corresponding to the growth of the solution.

In the one-dimensional case, we consider the problem:

$$u_t = au_{xx} \ \text{ for } \ x > 0, \ \ t > 0, \tag{1}$$

$$c_0u_t - u_x = f(u) \ \text{ for } \ x = 0, \ \ t > 0, \tag{2}$$

$$\lim_{x\to\infty} u(x,t) = u_\infty(t), \tag{3}$$

$$u(x,0) = u_0(x) \geq 0 \ \text{ for } \ x > 0; \ \ -u_0'(0) = f(u_0(0)). \tag{4}$$

I. Lirkov, S. Margenov, and J. Waśniewski (Eds.): LSSC 2005, LNCS 3743, pp. 509–517, 2006.

The function $f(u)$ often is positive and tends to infinity as $u \to \infty$. Thus, in heat flow interpretation, the condition (2) is an absorption law [14], which makes heat flow in the body (in the present paper the body is infinite), [2,14]. In [2,4,7,8], existence and nonexistence in large time of solutions of such problems are studied.

We also consider the two-dimensional problem

$$u_t = a\triangle u, \quad (x, y, t) \in \Omega = \{0 < x < l, y > 0, 0 < t < \infty\}, \tag{5}$$

$$u(0, y, t) = f_1(y, t), \quad u(l, y, t) = f_2(y, t), \quad y > 0, \quad 0 < t < \infty, \tag{6}$$

$$c_0 u_t - u_y = f(u),\ y = 0;\ \lim_{y\to\infty} u(x, y, t) = u_\infty(y, t),\ 0 < x < l, 0 < t < \infty, \tag{7}$$

$$u(x, y, 0) = u_0(x, y), \quad y \geq 0, \quad 0 < x < l, \tag{8}$$

where l, a and c_0 are real numbers, f, f_1 and f_2 are given functions. This problem in comparison with the one dimensional one is less studied.

The remainder part of this paper is organized as follows. In Section 2 we define QUM and present some derivative approximations. Also, we derive second order approximation with respect to x for problem (1)-(4) and formulate two theorems for convergence. For blow-up solutions we use decreasing variable time step. The numerical experiments, given in this section illustrate the efficiency of the algorithm. The next section is devoted to the two-dimensional problem (5)-(8). Finally, we give some conclusions.

2 The 1D Heat Problem (1)-(4)

In this section we will provide an $O(\tau + N^{-2})$ approximation to the solution of the continuous problem (1)-(4).

2.1 Quasi-uniform Mesh and Space Discretization

Definition 1. [1] *Let $x(\xi)$, $\xi \in [0, 1]$, $x \in [a, b]$ is strong monotone sufficiently smooth function. Then the mesh $w_N = \{x_i = x(\frac{i}{N}),\ 0 \leq i \leq N\}$ in $[a, b]$ we call quasi-uniform.*

We shall implement to our problems the meshes [1]

$$x(\xi) = -c\ln(1 - \xi), \quad h_0 = x_1 - x_0 \simeq \frac{c}{N}, \quad x_{N-1} = c\ln N, \tag{9}$$

$$x(\xi) = c\xi/(1 - \xi)^m, \quad h_0 =\simeq \frac{c}{N}, \quad x_{N-1} \simeq cN^m, \quad m > 0, \tag{10}$$

where $c > 0$ is controlling parameter. The choice of c is a result from the fact that the half of intervals are in domain with length $\sim c$. The last interval of (9) and (10), $[x_{N-1}, x_N]$, is infinite, but the point $x_{N-1/2}$ is finite, because the non integer nodes are given by $x_{i+\alpha} = x(\frac{i+\alpha}{N})$, $|\alpha| < 1$. Therefore, QUM transforms the infinite domain in to finite number of intervals and **states the original boundary condition directly on infinity**.

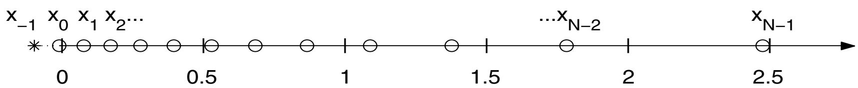

Fig. 1. Offset grid, QUM is (9), $N = 12$, $c = 1$, x_0 falls halfway between x_{-1} and x_1

We shall use the following derivative approximations

$$
\begin{aligned}
&(\frac{\partial u}{\partial x})_{i+1/2} \approx \frac{u_{i+1} - u_i}{2(x_{i+3/4} - x_{i+1/4})}, \\
&(\frac{\partial^2 u}{\partial x^2})_i \approx \frac{1}{x_{i+1/2} - x_{i-1/2}}[(\frac{\partial u}{\partial x})_{i+1/2} - (\frac{\partial u}{\partial x})_{i-1/2}].
\end{aligned}
\tag{11}
$$

The formulas contain $u_N = u_\infty(t)$**, but not** $x_N = \infty$. The truncation errors are of order $O(N^{-2})$. In order to obtain a second order approximation for the nonlinear boundary condition (2), we use an offset grid, see Figure 1.The point x_{-1}, outside of the domain, is fictitious. Using (11), and the second order approximation

$$
(\frac{\partial u}{\partial x})_0 \approx \frac{1}{2}[(\frac{\partial u}{\partial x})_{1/2} + (\frac{\partial u}{\partial x})_{-1/2}]
\tag{12}
$$

(with residual term $\frac{1}{N^2}[\frac{x_{\xi\xi\xi}}{6x_\xi}u_x + \frac{x_{\xi\xi}}{2}u_{xx} + \frac{(x_\xi)^2}{6}u_{xxx}] + O(N^{-4})$), we obtain the difference equation in the node $x_0 = 0$. After an implementation of the above derivative approximations (11),(12) in (1)-(4), we obtain the next ordinary differential equations system:

$$
\dot{z}_0 = \frac{2a}{H_0^1}[\frac{z_1 - z_0}{2H_0^2} - f(z_0)],
\tag{13}
$$

$$
\dot{z}_i = \frac{a}{H_i^1}[\frac{z_{i+1} - z_i}{2H_i^2} - \frac{z_i - z_{i-1}}{2H_i^3}], \quad i = 1, ..., N-1
\tag{14}
$$

$$
\dot{z}_N = u_\infty(t),
\tag{15}
$$

where $z_i = z(x_i) \approx u(x_i, t)$, $H_0^1 = 2x_{1/2}$, $H_i^1 = x_{i+1/2} - x_{i-1/2}$, $i = 1, ..., N-1$, $H_i^2 = x_{i+3/4} - x_{i+1/4}$, $H_i^3 = x_{i-1/4} - x_{i-3/4}$, $i = 0, ..., N$.

In problem (1)-(4) a reaction term $f(u)$ at the boundary is considered and if for example $f(u) = u^p$, $p > 1$, then blow-up phenomena occurs in the sense that there exist a finite time T, such that $\lim_{t \to T} \|u(.,t)\|_\infty = +\infty$ for convenient initial data [2,4,6-8,12]. Then, the solution of the semidiscrete problem (13)-(15) also blows-up in finite time T_h. For numerical approximations of blow-up problems on **bounded domains** we refer to [5,6,12,13], the survey [3] and the references therein. In the frame of the present work we are not able to discuss for our problems such interesting questions as convergence of T to T_h, when $N \to \infty$, asymptotic behavior of the semidiscrete numerical approximations, etc.

A remarkable (and well known fact) is that the solutions of parabolic problems with nonlinear boundary conditions develop blow-up regardless the smoothness of the initial data u_0, [2,4,6-8,12]. We assume that $u \in C^{4,2}((0,\infty),(0,\infty))$ and we shall call such solution **regular**.

Theorem 1. *Let u be a regular solution of (1)-(4) and z is it's numerical approximation given by (13)-(15). Then for $\forall\ 0 < \tau < T$ there exists a constant C, independent of N, such that*

$$\max_i \max_{0\le t\le T-\tau} |u(x_i,t) - z_i(t)| \le CN^{-2}.$$

This theorem also covers the case of global existence of regular solution to problem (1)-(4).

Theorem 2. *Let T and T_h be the blow up times for u and z respectively. Then $\lim\limits_{N\to\infty} T_h = T$.*

2.2 Time Discretization

We introduce a nonuniform mesh grid in time

$$t_0 = 0, \quad t_n = t_{n-1} + \triangle t_{n-1} = \sum_{k=0}^{n-1} \triangle t_n \quad (\triangle t_k \ge 0, k = 0,1,...).$$

The choice of the time step $\triangle t_n$ in the system (13)-(15) depends on the growth of the solution z, [3,13]. For the sake of simplicity, we take $f(u) = u^p$, $p > 0$. The time increment $\triangle t_n$ is chosen to be variable

$$\triangle t_n = \tau \times \min\{1, \frac{H_0^1 + 2ac_0}{2a\,\|z\|_{\infty(or2)}^{p-1}}\}, \quad \tau = \max_{0\le k\le n-1} \triangle t_k.$$

The full discretization of the problem (1)-(4), $f(u) = u^p \approx (z^n)^p z^{n+1}$, $i = 1,...,N-1$ is as follows:

$$\begin{aligned}
&[1 + \frac{a\triangle t_n}{H_0^1 + 2ac_0}(\frac{1 - 2(z_0^n)^{p-1}H_0^2}{H_0^2})]z_0^{n+1} - \frac{a\triangle t_n}{H_0^2(H_0^1 + 2ac_0)} z_1^{n+1} = z_0^n,\\
&-\frac{a\triangle t_n}{2H_i^1 H_i^3} z_{i-1}^{n+1} + (1 + \frac{a\triangle t_n}{2H_i^1}(\frac{1}{H_i^2} + \frac{1}{H_i^3}))z_i^{n+1} - \frac{a\triangle t_n}{2H_i^1 H_i^2} z_{i+1}^{n+1} = z_i^n, \qquad (16)\\
&z_N^{n+1} = u_\infty(t^{n+1}).
\end{aligned}$$

2.3 Computational Results

The aim of the numerical experiments is to show the convergence rate and to compare the accuracy of the algorithms, using QUM and ABCs (Example 1); also, to test the efficiency of both QUMs (9) and (10) (Example 2).

A method of ABCs, is presented in [16] for one-dimensional parabolic equation defined in semi-infinite interval with Dirichlet boundary condition at the left end. We developed this algorithm to the case of nonlinear (dynamical and Neumann) boundary conditions for 1D and 2D problems. The details are given in the submitted paper [11]. Here we draw the analogy between QUM method (16) (QUMM) and the exact artificial boundary method, [11], using QUM for computing the truncated problem (ABCQUMM). The approximation of ABC we derive in the same manner as for (2). The examples are chosen such that the construction of ABCs is possible in sense of [11,16], i.e. $u_\infty = 0$ and supp $u_0 < \infty$.

Example 1. The test problem is (1)-(4), where $f(u) = u^2 + \tilde{f}(t)$, $a = 1$, $u_0(x) \equiv 0$, $u_\infty = 0$, $\tilde{f}(t)$ is chosen such that the exact solution is $u(x,t) = \operatorname{erfc}(\frac{x+2}{2\sqrt{t}})$, $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int\limits_x^\infty e^{-\lambda^2} d\lambda$, $\tilde{f}(t)$ is different for $c_0 = 0$ and $c_0 = 1$. Let denote by E_∞^N ($E_\infty^N = \|E_i\|_c$) and E_2^N the errors in corresponding discrete max and L_2 norms, obtained using mesh with $N+1$ nodes. Instead of the standard error E_2^N, for method of QUM we use the estimate $E_2^N = [\frac{1}{2} H_0^1 (E_0)^2 + \sum\limits_{i=1}^{N-1} H_i^1 (E_i)^2]^{1/2}$. The ratio $\tau N^2 = 1$ is fixed. The computations are performed up to time $t = 1$ with QUM (9). The convergence rate (CR) is valued by the quantities $CR_{\infty(2)} = \log_2 [E_{\infty(2)}^N / E_{\infty(2)}^{2N}]$.

Having exact solution, we compare the efficiency of the algorithms, imposing the exact boundary condition in x_{N-1}: $u(x_{N-1}, t) = \operatorname{erfc}(\frac{x_{N-1}+2}{2\sqrt{t}})$ on QUM (DQUM). In Table 1 we give the results for the case of dynamical ($c_0 = 1$) boundary conditions. There is no essential difference with the case $c_0 = 0$. The computations confirm the efficiency of QUMM and it's convergence order 2. The approximation of ABC (ABCQUMM) uses the discrete values of the artificial boundary from all previous time levels. That's way, the accumulation of round off error is possible. Nevertheless, ABCQUUMM is more stable in time than QUMM. For example, at t=2: $E_\infty^{24} = 6.926715e-4$ for QUMM, $E_\infty^{24} = 3.063709e-4$ for ABCQUMM and $E_\infty^{24} = 1.526854e-4$ for DQUM.

For $\tilde{f}(t) \equiv 0$ the solution blows-up in finite time, [8]. Numerical experiments for such solutions are discussed in [11].

Table 1. Global errors in different norms, $c_0 = 1$, QUM is (9)

N	QUMM		ABCQUMM		DQUM	
	E_∞^N	E_2^N	E_∞^N	E_2^N	E_∞^N	E_2^N
12	3.683837e-4	3.523132e-4	3.687771e-4	3.79614902e-4	3.681274e-4	3.369317e-4
24	9.323924e-5	8.858261e-5	9.324177e-5	9.206816e-5	9.323728e-5	8.703128e-5
48	2.332366e-5	2.206979e-5	2.332367e-5	2.273758e-5	2.332365e-5	2.202332e-5
96	5.830883e-6	5.517726e-6	5.830883e-6	5.587760e-6	5.830883e-6	5.507968e-6
192	1.473248e-6	1.394342e-6	1.473248e-6	1.397895e-6	1.457999e-6	1.377982e-6

Example 2. We use QUM (10) for solving the problem from Example 1. All input datum are the same, except the mesh. We give the results in Table 2.The efficiency of (9) and (10), $m = 1$ are close for this problem.

Table 2. Global errors in different norms and convergence rate, $c_0 = 1$, QUM is (10)

N	$m=1$				$m=2$			
	E_∞^N	CR_∞	E_2^N	CR_2	E_∞^N	CR_∞	E_2^N	CR_2
12	3.236310e-4		2.604571e-4		4.526466e-4		4.588175e-4	
24	8.221002e-5	1.9770	6.501900e-5	2.0021	1.066523e-4	2.0855	1.165572e-4	1.9769
48	2.056667e-5	1.9990	1.627574e-5	1.9981	2.645880e-5	2.0111	2.909814e-5	2.0020
96	5.141504e-6	2.0000	4.069750e-6	1.9997	6.604643e-6	2.0022	7.273963e-6	2.0001
192	1.285694e-6	1.9996	1.017630e-6	1.9997	1.654158e-6	1.9974	1.817768e-6	2.0006

3 The 2D Heat Problem

In this section we construct second order (with respect to space variable) approximation of the differential problem (5)-(8) by QUMM.

3.1 Discretization of (5)-(8)

The mesh in x direction is classical: uniform grid with $M + 1$ nodes and mesh step size k, while in y direction we use QUM (9) or (10) with $N + 1$ mesh points, see Figure 2. As in the one-dimensional case, we use fictitious nodes: $M - 1$ numbers, situated under the bottom boundary, h_0 away. The elimination is standard. Using (11) for $\frac{\partial^2 u}{\partial y^2}$, central approximation for $\frac{\partial^2 u}{\partial x^2}$ and (12) for $\frac{\partial u}{\partial y}$, we obtain the following semidiscretization of the problem (5)-(8):

$$z_{0j} = f_{1_{0j}}, \qquad z_{Mj} = f_{2_{Mj}}, \qquad j = 1, ..., N-1, \tag{17}$$

$$z_{iN} = u_\infty(x_i, t), \qquad i = 1, ..., M, \tag{18}$$

$$\dot{z}_{ij} = \frac{a(z_{ij+1} - z_{ij})}{2H_j^2 H_j^1} - \frac{a(z_{ij} - z_{ij-1})}{2H_j^3 H_j^1} + \frac{a(z_{i+1j} - 2z_{ij} + z_{i-1j})}{k^2}, \tag{19}$$

$$\dot{z}_{i0} = \frac{aH_0^1 \left[z_{i+1,0} - 2z_{i0} + z_{i-1,0}\right]}{(H_0^1 + 2ac_0)k^2} + \frac{2a}{(H_0^1 + 2ac_0)} \left[\frac{z_{i1} - z_{i0}}{2H_0^2} + f(z_{i0})\right], \tag{20}$$
$$i = 1, ..., M-1, \qquad j = 1, ..., N-1.$$

Now, $z_{ij} = z(x_i, y_j) \approx u(x_i, y_j, t)$ and H_j^s, $s = 1, 2, 3$ are the same as in (13)-(15), but $x \leftrightarrow y$ $(i \leftrightarrow j)$.

Results of convergence, analogical to Theorem 1,2, hold for the 2D problem.

Remark 1. The QUMM can be applied without difficulties to the cases of more complicated boundary conditions. For example, if instead of $u(0, y, t) = 0$, we have $c_1 u_t - u_x = g(u)$, we will use $M + N$ fictitious nodes to obtain second order

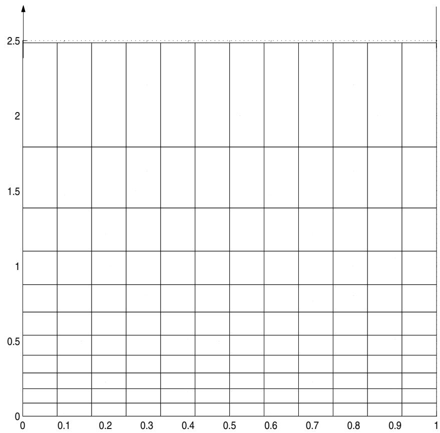

Fig. 2. QUM (9), N=M=12, $c = 1$

Table 3. Global errors in different norms and CR, $M = N$, $c_0 = 1$, QUM is (9)

N/CR	E_∞^N	E_2^N
12	4.058624e-3	2.070943e-3
24	1.084095e-3	5.283785e-4
CR	1.9045	1.9706
48	2.731855e-4	1.326197e-4
CR	1.9885	1.9943
96	6.864776e-5	3.318021e-5
CR	1.9926	1.9989
192	1.713742e-5	8.283924e-6
CR	2.0020	2.0019

approximation. For approximation of the solution in the corner node $x = 0$, $y = 0$ we use two fictitious nodes. Thus for $i = 0$ and $j = 0, ..., N-1$ we have

$$\dot{z}_{00} = \frac{2kaH_0^1}{kH_0^1 + 2a(c_1H_0^1 + c_0k)}\left[\frac{z_{10} - z_{00}}{k^2} + \frac{g(z_{00})}{k} + \frac{z_{01} - z_{00}}{2H_0^1H_0^2} + \frac{f(z_{00})}{H_0^1}\right],$$

$$\dot{z}_{0j} = \frac{2a}{k+2ac_1}\left[\frac{z_{1j} - z_{0j}}{k} + g(z_{0j})\right] + \frac{ak}{H_j^1(k+2ac_1)}\left[\frac{z_{0j+1} - z_{0j}}{2H_0^2} - \frac{z_{0j} - z_{0j-1}}{2H_0^3}\right].$$

Now, it's very easy to obtain the full discretization in the case $f(u) = u^p \approx (z^n)^{p-1}z^{n+1}$, $p > 1$ $(g(u) = u^q \approx (z^n)^{q-1}z^{n+1}$, $q > 1)$ by substituting $\dot{z}$ with $\frac{z^{n+1}-z^n}{\triangle t_n}$ and write all unknown values z on the $n+1-th$ time level.

The time step in (17)-(19) is chosen as follows

$$\triangle t_n = \tau \times \min\{1, \frac{H_0^2(H_0^1 + 2ac_0)}{a\left\|z\right\|_{\infty(or2)}^{p-1}}\}, \quad \tau = \max_{0\le k\le n-1} \triangle t_k.$$

3.2 Computational Results

Example 3. The test problem is (5)-(8), $f_1(y,t) = \operatorname{erfc}(\frac{y}{2\sqrt{t}})$, $f_2(y,t) = \operatorname{erfc}(\frac{l+y}{2\sqrt{t}})$, $u_\infty = 0$ and instead of (7), we impose $u(x,0,t) = \operatorname{erfc}(\frac{x}{2\sqrt{t}})$, $l = 1$, $a = 0.5$. The exact solution is $u(x,y,t) = \operatorname{erfc}(\frac{x+y}{2\sqrt{t}})$. The results are in Table 3 (L_2 error is on the analogy of 1D case), $t = 0.1$, $u_0 \equiv 0$, $\tau = [\min\{k, \min_{0\leq i\leq N-1} h_i\}]^2$. Obviously, the convergence rate is $O(\tau + k^2 + N^{-2})$. There is no qualitative difference with results, obtained by ABCQUMM.

4 Conclusions

In this paper we used the QUMM for solving 1D and 2D heat problems with nonlinear dynamical ($c_0 = 1$ or $c_1 = 1$) or Neumann ($c_0 = 0$ or $c_1 = 0$) boundary conditions. We draw the analogy between two algorithms: QUMM and ABC-QUMM. Both methods are with convergence order 2 in space and 1 in time and could be applied efficiently for solving problems, defined on unbounded domains. But it is easy to obtain higher order convergence rate, also with respect to time variable, using for example Crank-Nickolson (including half nodes), [16] or Rozenbrok-Vanner (two-step) schemes, see [1].

The efficiency of the QUMM is very close to those of the ABCQUMM. Indisputably, the most important advantage of the QUMM is that the method is easy applicable for a wide class of problems (including nonlinear problems).

Acknowledgments

This research is supported by Bulgarian National Fund of Science under Project HS-MI–106/2005.

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