Mathematica Balkanica

Mathematical Society of South-Eastern Europe
A quarterly published by
the Bulgarian Academy of Sciences – National Committee for Mathematics

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Mathematica
Balkanica

New Series Vol. 14, 2000, Fasc. 3-4

Method of Lines for Parabolic Equations with Dynamical Boundary Conditions

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In this paper one-dimensional parabolic problems that involve time derivative in the boundary conditions are solved using the method of lines (MOL). Factors influencing the choice of the ODEs solvers that results from the spatial discretization are investigated on the model advection - diffusion equation. Convergence of MOL schemes is proved. Numerical experiments confirm and complement the theoretical results.

AMS Subj. Classification: 65N40

Key Words: method of lines, ODE solvers, difference schemes

1. Introduction

The method of lines, MOL, is a well-known approach in the numerical solution of time-dependent partial differential equations (PDEs) with classical boundary conditions, i.e. Dirichlet, Neumann and Robbin conditions. In this approach the solution process is thought of as consisting of two parts, viz. the space discretization and the time discretization. By discretizing the space variable by finite differences, finite elements , spectral techniques, etc., the PDE is approximated by a system of ordinary differential equations (ODEs). Such a semidiscretization is often an intermediate step in the derivation of a fully discrete scheme, but in the MOL approach the ODEs are integrated directly with a standard code for the task.

In this article we analyse the MOL for problems of the following type:

$$\dot{u}(x,t) = f(x,t,u(x,t),u'(x,t),u''(x,t)) \ , \ 0 < x < 1, 0 < t < T < \infty, \tag{1.1}$$

$$\varepsilon_0 \dot{u}(0,t) = g_0(t,u(0,t),u'(0,t)) \ , \ 0 < t < T, \tag{1.2}$$

$$\varepsilon_1 \dot{u}(1,t) = g_1(t, u(1,t), u'(1,t)) \ , \ 0 < t < T, \tag{1.3}$$

$$u(x,0) = \varphi(x) \ , \ 0 \le x \le 1, \tag{1.4}$$

where $\varepsilon_0, \varepsilon_1$ are nonnegative constants; the time and space derivatives are denoted, respectively, by a dot and a prime. Our basic assumptions are:

$$\frac{\partial f}{\partial u''} \ge D > 0, \tag{1.5}$$

$$\frac{\partial g_0}{\partial u'} \ge D_0 > 0 \ , \ \frac{\partial g_1}{\partial u'} \le D_1 < 0. \tag{1.6}$$

Therefore, the problem (1.2)-(1.4) is parabolic. One observes that when $\varepsilon_0 > 0$ or $\varepsilon_1 > 0$ (or both), the boundary conditions are non-standard since (1.2), (1.3) involve derivatives with respect to the time. Such conditions are called dynamic (nonstationary) boundary conditions (D.B.Cs.), [2, 6]. Problems of type (1.1)-(1.4) are used to describe mathematical models in the theory of heat conduction, chemical reaction theory and colloid chemistry; see the survey and references in [2].

We also refer to [2], where a phenomenologial deduction of semilinear problems of type (1.1)-(1.4) is given. There a diffusion process is considered in the solid $\Omega = (0,1)$ placed in a fluid or a gas. The transport equation is

$$\dot{u}(x,t) - (p(x,t)u'(x,t))' = f(u(x,t)) \text{ in } \Omega \times (0,T). \tag{1.7}$$

Here

$$p(x,t) \ge p_0 > 0 \tag{1.8}$$

represents the diffusion coefficient (or thermal conductivity), the scalar field pu' is the heat flux, $f(u(x,t))$ stands for some source term and $\varepsilon_0 > 0$ or ε_1 (or both) mean(s), that the left boundary $x = 0$ (respectively right $x = 1$) (or both) of the body Ω are permeable to heat and we obtain the DBCs:

$$\varepsilon_0 \dot{u}(0,t) - p(0,t)u'(0,t) = g_0(u(0,t)) \ , \ 0 < t < T, \tag{1.9}$$

$$\varepsilon_1 \dot{u}(1,t) + p(1,t)u'(1,t) = g_1(u(1,t)) \ , \ 0 < t < T, \tag{1.10}$$

$$u(x,0) = \varphi(x) \ , \ 0 \le x \le 1. \tag{1.11}$$

When $\varepsilon_0 = 0$ or $\varepsilon_1 = 0$ (or both), the corresponding boundary is impervious to heat and we get the classical Robbin BCs.

The problem (1.7) - (1.10) with $f \equiv 0, g_0 \equiv 0$ and $u(1,t) = 0$ instead of (1.10), is considered by Samarskii [7, p.396]. There, a fully discrete scheme with weight γ, $0 \leq \gamma \leq 1$, which has $0(r^{m_\gamma} + h^2)$ local truncation error, where r and h are the time and space steps discretizations, respectively, and

$$m_\gamma = 2 \text{ if } \gamma = 0.5 \ , \ m_\gamma = 1 \text{ if } \gamma \neq 0.5,$$

is constructed. Realization and convergence of this scheme are also studied.

In Section 2 the phenomenon stiffness which is invariable property associated with the process of solving the ODEs is discussed. Also, a result of Verwer and Sanz-Serna for the convergence of MOL is prepared for applications. In this paper several semidiscrete schemes for solving problems (1.1)-(1.4), (1.7)-(1.10) are studied. First, in Section 3 prototypes of these schemes are analysed for the advection-diffusion equation. This analysis throws light on the choice of ODE solvers for the numerical solution of the nonlinear problems (1.1)-(1.4), (1.7)-(1.10). Then, in Section 4, this study is generalized to the nonlinear PDEs in question. Also, equation (1.7) is approximated by finite differences with $O(h^2)$ local trunctation error as $h \to 0$ at the interior mesh points $h, \ldots, nh$, and equations (1.8),(1.9) - with $O(h)$ local truncation error at the points 0 and $1 = (n+1)h$, respectively. Realistic numerical examples which confirm and complement the theoretical conclusions in previous sections are presented in Section 5.

2. Preliminaries

For integer n we denote $h = 1/(n+1)$ and approximate $u(kh,t)$ by $y_k(t)$ for $k = 0, 1, \ldots, n+1$. The approximations (see Section 3) to problems (1.1)-(1.4),(1.7)-(1.11) are ODEs of the form:

$$\dot{y}(t) = F(t, y(t)) \ , \ y(0) = \varphi(0), \tag{2.1}$$

$$y(t) = [y_0(t), \ldots, y_{n+1}(t)]^T, \ \varphi(0) = (\varphi(0), \ldots, \varphi(kh), \ldots, \varphi(1))^T.$$

The first goal of the present paper is to analyse numerical solution of the ODEs (2.1). The system (2.1) is said to be stiff, if the eigenvalues $\lambda_0, \ldots, \lambda_{n+1}$ of the Jacobian matrix J satisfy the relation

$$\max_k [|Re(\lambda_k)|] \gg \min_k [|Re(\lambda_k)|].$$

The ratio

$$S(t) = \frac{\max_k [Re|\lambda_k|]}{\min_k [Re|\lambda_k|]}$$

is called stiffness ratio of the system [1, 4, 8].

The second goal is the treatment of the semidiscrete approximations convergence for equations (1.1)-(1.3) and (1.7)-(1.9) in the class of "bounded" nonlinearities. We apply the following results of Verwer and Sanz-Serna [11]. The vector $u_h(t) = (u(0,t), \dots, u(kh,t), \dots, u(1,t))^T$ satisfies (2.1) with a residual $r(t)$ that is the truncation error of the spatial difference approximations

$$r(t) = F(t, u_h(t)) - \dot{u}_h(t).$$

A discretization is said to be consistent, if there is a norm for which $\|r(t)\| \to 0$ uniformly in t as $h \to 0$. The error of the semidiscrete approximation is $\eta(t) = y(t) - u_h(t)$. Using the mean value theorem for vector functions, it is found that

$$\dot{\eta} = \mu(t)\eta + r(t),$$

where

$$\mu(t) = \int_0^1 \frac{\partial}{\partial y} F(t, u_h + \theta\eta)d\theta.$$

The convergence follows from an inequality that bounds $\|\eta\|$ in terms of a bound on $\|r\|$ and a factor depending on a bound for the logarithmic norm corresponding to the chosen norm $\|.\|$.

R e m a r k . The *logarithmic norm* of the matrix A is the number $\mu[A] = \lim_{h \to 0+} \frac{\|E+hA\|}{h}$, where E is the identity matrix.

In L_∞ the norm of a vector $v = (v_1, v_2, \dots, v_n)$ and the corresponding norm of a matrix $A = (a_{ij})_{,i,j=1,2,\dots,n}$ are given by

$$\|v\|_\infty = \max_{1 \le i \le n} |v_i| \ , \ \|A\|_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}| \ . \tag{2.2}$$

The L_1 norms are defined by

$$\|v\|_1 = \sum_{i=1}^{n} |v_i| \ , \ \|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{n} |a_{ij}| \ . \tag{2.3}$$

The L_∞ and L_1 *logarithmic norms* of a matrix corresponding to (2.2) and (2.3) are given by

$$\mu_\infty[A] = \max_{1 \le i \le n} (a_{ii} + \sum_{j=1, j \ne i}^{n} |a_{ij}|) \ ,$$

$$\mu_1[A] = \max_{1\leq j\leq n} (a_{jj} + \sum_{i=1,i\neq j}^{n} |a_{ij}|) \,.$$

Let $T_h(t) = u_h(t) + \theta\eta(t), 0 \leq \theta \leq 1$, and let μ_{max} be a constant such that

$$\mu_{max} \geq max_\varsigma \mu[\frac{\partial}{\partial y}F(t,\varsigma)] : \varsigma \in T_h(t) \; for \; all \; t \in [0,T].$$

If $\|\eta(0)\| = 0$, it follows that

$$\|\eta(t)\| \leq C(t,\mu_{max}) max \|r(\tau)\| \; for \; 0 \leq t \leq T,$$

where $C(t,\mu_{max}) = (exp(\mu_{max}t) - 1)/\mu_{max}$.The conclusion is the following theorem, [11].

Theorem 1. *Suppose that the discretization is consistent and that* μ_{max} *exists independent of the mesh spacing. Then* $\|y(t) - u_h(t)\| \to 0$ *as* $h \to 0$*, i.e., the MOL converges. If the truncation error is* $O(h^p)$ *uniformly for* $0 \leq t \leq T$*, the error* $\|y(t) - u_h(t)\|$ *is also* $O(h^p)$.

3. Linear problem

The advection-diffusion equation

(3.1) $$\dot{u}(x,t) - Du''(x,t) + \nu u'(x,t) = 0$$

has often been used for the study of numerical methods for the solution of PDEs. We shall solve (3.1) with DBCs,

(3.2) $$\varepsilon_0 \dot{u}(0,t) - Du'(0,t) = -g_{00}(t)u(0,t) + g_{01}(t),$$

(3.3) $$\varepsilon_1 \dot{u}(1,t) + Du'(1,t) = -g_{10}(t)u(1,t) + g_{11}(t).$$

In this section, we assume that $D \geq 0$, $\nu \geq 0$ and additionally - $g_{00}(t) \geq 0$, $g_{10}(t) \geq 0$. We shall approximate the partial derivatives with respect to x in (3.1) by central derivatives

(3.4) $$\dot{y}_k = D\frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} - \nu\frac{y_{k+1} - y_{k-1}}{2h}, \quad k = 1,\ldots,n.$$

3.1. $O(h)$ approximation of the BCs

Consider one-sided difference approximations to the D.B.Cs:

$$\varepsilon_0 \dot{y}_0 = D\frac{y_1 - y_0}{h} - g_{00}(t)y_0 + g_{01}(t), \tag{3.5}$$

$$\varepsilon_1 \dot{y}_{n+1} = -D\frac{y_{n+1} - y_n}{h} - g_{10}(t)y_{n+1} + g_{11}(t). \tag{3.6}$$

We group the approximations as a vector $y = (y_0, \ldots, y_{n+1})^T$ and write the equations (3.4)-(3.6) as a linear, constant coefficient system of the form (2.1), namely:

$$\dot{y} = F(t, y) \equiv Jy + s(t), \tag{3.7}$$

where $\partial F/\partial y = J$ is a tridiagonal matrix with

$$J_{00} = -\frac{D}{\varepsilon_0 h} - \frac{1}{\varepsilon_0}g_{00}(t)\ ,\ J_{01} = \frac{D}{\varepsilon_0 h},$$

$$J_{k,k-1} = \frac{D}{h^2} + \frac{\nu}{2h}\ ,\ J_{k,k} = -2\frac{D}{h^2}\ ,\ J_{k,k+1} = \frac{D}{h^2} - \frac{\nu}{2h}\ ,\quad k = 1, \ldots, n$$

$$J_{n+1,n} = \frac{D}{\varepsilon_1 h}\ ,\ J_{n+1,n+1} = -\frac{D}{\varepsilon_1 h} - \frac{1}{\varepsilon_1}g_{10}(t)$$

and the inhomogeneous term is:

$$s(t) = (\frac{1}{\varepsilon_0}g_{01}(t), 0, \ldots, 0, \frac{1}{\varepsilon_1}g_{11}(t)).$$

The Jacobian of a system of ODEs plays a key role in establishing convergence and in selecting an appropriate integrator. In our case the mesh, or cell, and the Reynolds number $R = \nu h/D$ are important. If $R \leq 2$, then $J_{k-1,k}\ J_{k,k-1} > 0$ and J is quasi-symmetric. Further,

$$J_{00} + |J_{01}| = -g_{00}(t) \leq 0,$$

$$J_{n+1,n} + |J_{n+1,n+1}| = -g_{10}(t) \leq 0,$$

$$J_{k,k} + |J_{k,k-1}| + |J_{k,k+1}| = 0.$$

These observations imply that $\mu_\infty[J] = 0$ and, as a consequence from Theorem 1, the convergence follows. A standard result about the logarithmic norm ([1],p. 31) is: if λ is any eigenvalue of the matrix A, then $Re(\lambda) \leq \mu_\infty[A]$.

Since J is quasi-symmetric, then all the eigenvalues are real. Therfore, all eigenvalues of J are non-positive. Also, a well-known result about symmetric and quasi-symmetric matrix A is: if $\lambda_0 \leq \ldots < \lambda_{n+1}$ are the eigenvalues of A, then for all k, $\lambda_0 \leq A_{kk} \leq \lambda_{n+1}$. A typical entry on the diagonal of J is $-2Dh^{-2}$, which tells us that some of the eigenvalues have negative real part of magnitude $O(h^{-2})$; hence the system (2.7) is stiff for solutions that are easy to approximate. In view of the expression for J_{00} (or $J_{n+1,n+1}$), this system is much stiffer when ε_0 (respectively, ε_1) is small in comparison with h, i.e. $\varepsilon_0 \ll h$.

When the advection dominates ($R \geq 2$) and all or some of the eigenvalues are complex with large imaginary parts, then equation (3.1) assumes a hyperbolic character. In this case the system (2.1) is oscillatory and the methods efficient for stiff ODEs are not suitable for integration.

Using MATLAB, the eigenvalues of the Jacobian for small and large n are computed. The numerical values of the eigenvalues in dependence on n and $\varepsilon_0 = \varepsilon_1 \in (0, 1]$ are displayed in Tables 1 and 2. All the eigenvalues are complex with negative real parts. Note that Reynold's number is $R = 2 + \frac{1}{n+1}$ and in all the experiments $D = 1$ and $\nu = 2n - 1$ are assumed.

N	$m = \min\|Re\lambda_i\|$	$M = \max\|Re\lambda_i\|$	$s = \frac{M}{m}$
100	$9.949947 * 10^{-1}$	$3.295001 * 10^{4}$	$3.11159 * 10^{4}$
500	$9.989949 * 10^{-1}$	$9.633134 * 10^{5}$	$0.96427 * 10^{6}$

Table 1. $\varepsilon_0 = \varepsilon_1 = 1$

N	$m = \min\|Re\lambda_i\|$	$M = \max\|Re\lambda_i\|$	$s = \frac{M}{m}$
100	$6.648009 * 10^{1}$	$3.269566 * 10^{4}$	$4.91811 * 10^{2}$
500	$9.089931 * 10^{1}$	$9.635773 * 10^{5}$	$1.06005 * 10^{4}$

Table 2. $\varepsilon_0 = \varepsilon_1 = 10^{-2}$

If $\varepsilon_0 = \varepsilon_1 \to 0$ in (3.2) and (3.3), then Robin's boundary conditions are obtained. Therefore, Tables 1 and 2 show that the parabolic problems with DBCs are more stiff in comparison with those with classical BCs. Thus, many of the popular codes for stiff ODEs may be used [4], [5], [9], [10].

3.2. $O(h^2)$ approximations of the BCs

An $O(h^2)$-approximation of the left boundary condition can be obtained introducing a fictious mesh unknown y_{-1}:

$$\varepsilon_0 \dot{y}_0 = D\frac{y_1 - y_{-1}}{2h} - g_{00}y_0 + g_{01}$$

which is combined with (3.4), $k = 1$, for eliminating y_{-1}.Then

$$J_{00} = -\frac{D^2h^{-3} + g_{00}(Dh^{-2} + 0.5\nu h^{-1})}{k_0}\ , \quad J_{01} = \frac{D^2h^{-3}}{k_0},$$

$$k_0 = 0.5Dh^{-1} + \varepsilon_0(Dh^{-2} + 0.5\nu h^{-1}).$$

It is easy to see that $J_{01} > 0$ and J is quasi-symmetric for all h. Also

$$J_{00} + J_{01} \leq 0$$

for all h, when $g_{00} \geq 0$, so $\mu_\infty[J] = 0$. This implies convergence as $h \to 0$, and an error that is $O(h^2)$. Also, $k_0 = O(h^{-1})$ if $\varepsilon_0 = 0$, $k_0 = O(h^{-2})$, when $\varepsilon_0 = 1$.

Another $O(h^2)$ approximation makes use of Taylor's formula with equations (3.1), (3.2) to obtain

$$u'(0,t) = \frac{u_{x,0}}{1+0.5R} - \frac{h}{2D(1+0.5R)}\dot{u}(0,t) + 0(h^2).$$

Then, substituting this expression in (3.2) and omitting $O(h^2)$ terms, we obtain the following $O(h^2)$-approximation

$$\dot{y}_0 = \frac{D}{h(h+2\varepsilon_0(1+2R))}y_1 - \frac{D+2h(1+2R)g_{00}(t)}{h(1+2\varepsilon_0(1+2R))}y_0 + 2(1+2R)g_{01}(t).$$

A similar formula is valid for the right DBC (1.3).

A simple $O(h^2)$- approximation of the BCs (3.2), (3.3) is a second-order one-sided approximation to the space derivative in the BCs:

$$\varepsilon_0 \dot{y}_0 = D\frac{-y_2 + 4y_1 - 3y_0}{2h} - g_{00}(t)y_0 + g_{01}(t)$$

$$\varepsilon_1 \dot{y}_{n+1} = -D\frac{3y_{n+1} - 4y_n + y_{n-1}}{2h} - g_{10}(t)y_{n+1} + g_{11}(t).$$

The Jacobian is pentdiagonal with

$$J_{00} = \frac{1}{\varepsilon_0}(-\frac{3D}{2h} - g_{00})\ , \quad J_{01} = \frac{2D}{\varepsilon_0 h}\ , \quad J_{02} = -\frac{D}{2\varepsilon_0 h},$$

$$J_{n+1,n-1} = -\frac{D}{2\varepsilon_1 h}\ , \ J_{n+2,n} = \frac{2D}{\varepsilon_1 h}\ , \ J_{n+1,n+1} = \frac{1}{\varepsilon_1}(-\frac{3D}{2h} - g_{10}).$$

Similar numerical experiments by the help of MATLAB have been done for the eigenvalues of the Jacobians resulting from the both described $O(h^2)$ BCs approximations. They show that the behaviour of eigenvalues remains the same as indicated in Tables 1 and 2.

The following particular case confirms analytically the numerical results presented in details at the end of Subsection 3.1. By the assumption that in (3.1) $\nu = 0$, on the left boundary is stated a zero Dirichlet boundary condition (thus the number of unknowns becomes $n+1$) and on the right one - the dynamical boundary condition (1.10), the eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots < \lambda_{n+1}$ are found to be ([12]) $\lambda_k = \sin^2 \frac{\alpha_k h}{2}$, $k = 1, 2, \ldots, n+1$, where λ_k are the first $n+1$ positive roots of the equation $\cot \alpha = \frac{2}{h} \tan \frac{\alpha h}{2}$. This allows an estimate for the ratio $\frac{\lambda_{n+1}}{\lambda_1}$ to be obtained. It can be easily shown that $\frac{\lambda_{n+1}}{\lambda_1} \approx \frac{\alpha_{n+1}}{\alpha_1}$ and as $(k-1)\pi \leq \alpha_k \leq (k-1)\pi + \frac{\pi}{2}$ this leads to $S(t) = O(4n^2)$. Thus the degree of stiffness largely depends on the nature of the problem and the fineness of the spatial discretization used.

4. Nonlinear problems

In this section we develop our analysis of the linear equations (3.1) - (3.3), to the numerical solutions of the nonlinear problems (1.1) - (1.4), (1.7) - (1.11).

4.1. The general case

It is natural to expect that under some reasonable assumption on the nonlinear functions f, g_0, g_1, the behaviour of the numerical solutions of problem (1.1)-(1.4) will be similar to those of problem (3.1)-(3.3). Since by the considerations below the parameters ε_0, ε_1 are fixed, we put $\varepsilon_0 = \varepsilon_1 = 1$.

The simplest approximation of (1.1)-(1.4) gives the following ODEs:

$$\dot{y}_0 = g_0(t, y_0, \frac{y_1 - y_0}{2h}), \tag{4.1}$$

$$\dot{y}_k = f(x_k, t, y_k, \frac{y_{k+1} - y_{k-1}}{2h}, \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2}), \quad k = 1, \ldots, n, \tag{4.2}$$

$$\dot{y}_{n+1} = g_1(t, y_{n+1}, \frac{y_{n+1} - y_n}{h}), \tag{4.3}$$

with initial conditions $y_k(0) = \varphi(x_k), k = 0, \ldots, n+1$.

We shall make the following assumption for boundeness of the nonlinearities in the right-hand side of the problem (1.1)-(1.3):

(B) For all relevant arguments, $|\partial f/\partial u'|$, $|\partial g_0/\partial u'|$, $|\partial g_1/\partial u'|$ are bounded and there are constants k_0, k, k_1 such that

$$\partial g_0/\partial u \leq k_0 \ , \ \partial f/\partial u \leq k \ , \ \partial g_1/\partial u \leq k_1. \tag{4.4}$$

Theorem 2. *Let conditions (1.5), (1.6) and those in (B) be fulfilled. Then the semidiscrete approximation (4.1) - (4.3) of the problem (1.1) - (1.4) converges on any finite interval* $0 \leq t \leq T$ *and the truncation error is* $0(h)$. *When* $k_0, k, k_1 \leq 0$ *there is convergence for all* t. *Also, for a sufficiently small mesh spacing* h *the system of ODEs (4.1) - (4.3) is stiff.*

Proof. The equations (4.1) - (4.3) are assembled as a vector system $\dot{y} = F(t, y)$ of $n+2$ equations. The Jacobian $J = \partial F/\partial U$ is a tridiagonal matrix with

$$J_{00} = -\frac{1}{h}\frac{\partial g_0}{\partial u'} + \frac{\partial g_0}{\partial u} \ , \ J_{01} = \frac{1}{h}\frac{\partial g_0}{\partial u'},$$

$$J_{kk} = -\frac{2}{h^2}\frac{\partial f}{\partial u''} + \frac{\partial f}{\partial u},$$

$$J_{k,k\pm 1} = \frac{1}{h^2}\frac{\partial f}{\partial u''} \pm \frac{1}{2h}\frac{\partial f}{\partial u'} \ , \quad \text{for } k = 1, \ldots, n,$$

$$J_{n+1,n} = -\frac{1}{h}\frac{\partial g_1}{\partial u} \ , \ J_{n+1,n+1} = \frac{1}{h}\frac{\partial g_1}{\partial u'} + \frac{\partial g_1}{\partial u}.$$

The off-diagonal entries are positive and the matrix is quasi-symmetric, if

$$|\frac{\partial g_0}{\partial u'}| < \frac{D}{h}(\leq \frac{1}{h}\frac{\partial g_0}{\partial u'}),$$

$$|\frac{\partial f}{\partial u'}| \leq \frac{2D}{h}(\leq \frac{2}{h}\frac{\partial f}{\partial u''}),$$

$$|\frac{\partial g_1}{\partial u'}| < \frac{D}{h}(\leq \frac{1}{h}\frac{\partial g_1}{\partial u'})$$

for all components. Because of our assumptions about the boundedness of $|\partial g_0/\partial u|$, $|\partial g_1/\partial u|, |\partial f/\partial u'|$ and the positivity of D, this will certainly be true for all sufficiently small h. When it is true,

$$J_{00} + |J_{01}| \leq \frac{\partial g_0}{\partial u},$$

$$J_{kk} + |J_{k,k-1}| + |J_{k,k+1}| \leq \frac{\partial f}{\partial u}, \quad \text{for } k = 1, \ldots, n, \tag{4.5}$$

$$J_{n+1,n+1} + |J_{n,n+1}| \leq \frac{\partial g_1}{\partial u}.$$

In view of (4.5) we see now that $\max(k_0, k, k_1)$ is a bound on the logarithmic norm of the local Jacobian. Therefore, Theorem 1 applies, and establishes convergence on any finite time interval $0 \leq t \leq T$. When $k_0, k, k_1 \leq 0$, there is convergence for all t. With one-sided difference approximations in the BCs, the truncation error for smooth solutions is $O(h)$, so that the error of the approximate solution is $O(h)$.

Because the local Jacobian is quasi-symmetric, the eigenvalues are all real. For small mesh spacing h, the following inequalities hold:

$$\lambda_0 \leq J_{kk} = -\frac{2}{h^2}\frac{\partial f}{\partial u''} + \frac{\partial f}{\partial u} \leq -\frac{2D}{h^2} + k = O(h^{-2}),$$

$$\lambda_{n+1} \geq J_{00} = -\frac{1}{h}\frac{\partial g_0}{\partial u'} + \frac{\partial g_0}{\partial u} = O(h^{-1}). \tag{4.6}$$

When $k_0, k_1, k \leq 0$, the logarithmic norm of J is nonpositive and all eigenvalues are nonpositive. Then, it follows from (4.6) that the system of ODEs that arise from MOL is stiff for all sufficiently small mesh spacing h. The proof is completed. ■

When some of k_0, k or k_1 are positive, the matter is more complex. In such a situation eigenvalues with positive real parts appear, hence the solutions of ODEs grow as $exp(\rho t)$, $\rho > 0$. Shampine [10, pp. 749-750] discussed this case using an argument of Gear [4, p.213]. The conclusion is that the system of ODEs arising from the MOL is also stiff for sufficiently small spacing h.

4.2. The physical model

We continue to discuss the properties of the protype difference schemes in (4.1) and (4.2) on the physical problem (1.7) - (1.10). Let us begin with the approximation

$$\varepsilon_0 \dot{y}_0 = p(0,t) L'_h y_1 + g(y_0), \tag{4.7}$$

$$\dot{y}_k = L''_{h,p} y_k + f(y_k), \quad k = 1, \ldots, n, \tag{4.8}$$

$$\varepsilon_1 \dot{y}_{n+1} = -p(1,t) L'_h y_{n+1} + g_1(y_{n+1}), \tag{4.9}$$

where

$$L'_h z_k = \frac{z_k - z_{k-1}}{h}, \quad k = 1, n+1,$$

$$L''_{h,p} z_k = \frac{p_{k-0.5} z_{k-1} - (p_{k-0.5} + p_{k+0.5}) z_k + p_{k+0.5} z_{k+1}}{h^2},$$

$$p_{k-0.5} = p(x_k - 0.5h), \; p_{k+0.5} = p(x_k + 0.5h), \quad k = 1, \ldots, n.$$

Assuming that $p(x,t)$ is three times and $u(x,t)$ is four times continuously differentiable with respect to x, the local truncation error $\Phi_k(h,t)$ of the semidiscrete scheme (4.7)-(4.9) satisfies the inequalities

$$|\Phi_k(h,t)| = |L' u_k - u'(x_k,t)| \leq TCh, \quad \text{if } k = 0, n+1,$$

$$|\Phi_k(h,t)| = |L''_{h,p} u_k - (p(x_k,t) u'(x_k,t))'| \leq TCh^2, \quad \text{if } \; k = 1, \ldots, n,$$

where C is a constant independent on h.

Now, from Theorem 2 it follows the next corollary.

Corollary. *Let the conditions (1.8) and (4.4) be fulfilled. If* $p(0,t)$, $p(1,t)$, $p'(x,t)$, $0 \leq x \leq 1$ *are bounded on the interval* $0 \leq t \leq T$, *then the semidiscretization (4.7)-(4.9) converges on* $0 \leq t \leq T$ *and the truncation error is* $O(h)$. *When* $k_0, k, k_1 \leq 0$ *on* $0 \leq t \leq T$ *and* $p(0,t), p(1,t), p'(x,t)$ *are bounded for all* t, *there is convergence for all* t.

5. Numerical examples

Several properties of the theoretical discussion in the previous sections can be observed in numerical experiments. In particular, with the numerical examples we want to consider the following properties.

First, it is demonstrated that the implicit Runge-Kutta method of order 5 is more efficient than the diagonally implicit Runge-Kutta method of order 4. When the solution varies rapidly for both methods we use solvers RADAU5 and SDIRK4, respectively, described in [5].

Example 5.1.

The following problem is solved numerically:

$$\dot{u}(x,t) - \frac{4}{\pi^2} u''(x,t) = 0, \; 0 < x < 1, \; 0 < t < T \leq \infty,$$

$$u(x,0) = \sin\frac{\pi x}{2} + 1,$$

$$\dot{u}(0,t) - \frac{4}{\pi^2}u'(0,t) = -\frac{2}{\pi}e^{-t}u^3(0,t),$$

$$\dot{u}(1,t) + \frac{4}{\pi^2}u'(1,t) = 1 - u(1,t).$$

The analytic solution is

$$u(x,t) = e^{-t}\sin\frac{\pi x}{2} + 1.$$

The numerical results are displayed in Table 1, which contains the following information:

NFCN	Number of function evaluations,
NJAC	Number of Jacobian evaluations,
NDEC	Number of LU-decompositions of both matrces,
NACCPT	Number of accepted steps,
Error	The error at each t was measured by:

$$Error(t) = [\int_0^1 (y_k(t) - u(kh,t))^2 dt]^{\frac{1}{2}} \approx [h\sum_{k=0}^{n+1}(y_k(t) - u(kh,t))^2]^{\frac{1}{2}}.$$

All the experiments use relative error tolerance $TOL = 10^{-5}$.

T	h	RADAU5 / SDIRK4				
		NFCN	NJAC	NDEC	NACCPT	Error
0.1	10^{-1}	31	1	7	7	$0.1160 * 10^{-3}$
		36	2	10	10	$0.1179 * 10^{-3}$
	$\frac{1}{3}.10^{-2}$	31	1	7	7	$0.1203 * 10^{-6}$
		65	2	10	10	$0.5835 * 10^{-5}$
5	10^{-1}	172	15	21	22	$0.2080 * 10^{-3}$
		314	15	26	29	$0.2108 * 10^{-3}$
	$\frac{1}{3}.10^{-2}$	162	15	21	21	$0.1446 * 10^{-5}$
		310	15	24	29	$0.1986 * 10^{-5}$
30	10^{-1}	693	47	79	54	$0.2088 * 10^{-5}$
		659	44	70	60	$0.2223 * 10^{-5}$
	$\frac{1}{3}.10^{-2}$	687	48	81	54	$0.2515 * 10^{-6}$
		638	48	72	62	$0.1610 * 10^{-5}$

Table 3.

The second example confirms the conclusion of the second part of Theorem 3.

Example 5.2.

$$\dot{u}(x,t) - \frac{4}{\pi^2}u''(x,t) = 0,$$

$$u(x,0) = \sin\frac{\pi\varepsilon x}{2} + 1,$$

$$\varepsilon\dot{u}(0,t) - \frac{4}{\pi^2}u'(0,t) = -\frac{2\varepsilon}{\pi}e^{-\varepsilon^2 t}u^3(0,t),$$

$$\varepsilon\dot{u}(1,t) - \frac{4}{\pi^2}u'(1,t) = e^{-\varepsilon^2 t}(-\varepsilon^3\sin\frac{\pi\varepsilon}{2} + \frac{2\varepsilon}{\pi}\cos\frac{\pi\varepsilon}{2}).$$

The exact solution is

$$u(x,t) = e^{-\varepsilon^2 t}\sin\frac{\pi\varepsilon x}{2} + 1.$$

For the results see Table 4; compare with Table 3.

T	h	RADAU5				
		NFCN	NJAC	NDEC	NACCPT	Error
0.1	10^{-1}	28	1	7	7	$0.512 * 10^{-6}$
	$\frac{1}{3}.10^{-2}$	28	1	7	7	$0.264 * 10^{-13}$
1.0	10^{-1}	35	1	8	8	$0.184 * 10^{-5}$
	$\frac{1}{3}.10^{-2}$	32	1	8	8	$0.752 * 10^{-13}$
5.0	10^{-1}	39	1	9	9	$0.236 * 10^{-5}$
	$\frac{1}{3}.10^{-2}$	36	1	9	9	$0.768 * 10^{-13}$

Table 4. $\varepsilon = h$

MOL is sufficiently effective for numerical integration of parabolic problems with rapidly varying solutions or at long-time integration (see Table 3) along the asymptotic solutions. The next numerical experiment gives an insight into some open theoretical questions, namely - are there blow-up phenomena and what is the blow-up set S?

Example 5.3.

$$\begin{array}{ll} u_t = u_{rr} + \frac{1}{r}u_r + (u+1)^2 & \text{in } (0,1)\times(0,\infty) \\ u(r,0) = 1 & , r \in (0,1) \\ u_r = 0 & , r = 0 \\ \varepsilon.u_t + c_1.u_r = -c_2 u & , r = 1,\ \varepsilon \geq 0\ ,\ c_1 \geq 0\ ,\ c_2 \geq 0. \end{array}$$

In the case $\varepsilon = 0$ in $[3, x5.2]$, it is proved the following:
(i) if $c_2 = 0$ and $u(r,0) = const > 0$, then $S = [0,1]$,

(ii) otherwise $S = 0$.

Our numerical experiments are in agreement with this theoretical result. The result concerning (i) is displayed in Table 5. It is easily seen that near the blow-up time MOL is not sufficiently exact. For better calculating the blow-up solution specialized algorithms with variable time-step similar to those in [7] will be of a great help. This is a subject of a next paper.

RADAU5				
T	h	$u(x_0), x_0 = 0$	$u(x_1), x_1 = h$	$u(x_N), x_N = 1$
0.5	$\frac{1}{3}.10^{-3}$	$.57848591 * 10^8$	$.57848573 * 10^8$	$.57302637 * 10^8$
0.5000000177		$.36619761 * 10^{18}$	$.18721881 * 10^{15}$	$.60717356 * 10^{10}$

Table 5. $c_1 = 1$, $c_2 = 0, \varepsilon = 0$

The numerical results when $\varepsilon = 1$ are given in Tables 6 and 7. They show that when there is a dynamical boundary condition, the blow-up set is $S = 0$.

RADAU5					
T	h	$u(x_0), x_0 = 0$	$u(x_1), x_1 = h$	$u(x_N), x_N = 1$	$CPUTime, Sec$
1.960500	10^{-3}	$0.21018412 * 10^5$	$0.21000112 * 10^5$	0.14169260	
1.960551		$0.35845243 * 10^{15}$	$0.51029403 * 10^8$	0.14168536	1369.5055
1.971400	$\frac{1}{5}.10^{-3}$	$0.15663673 * 10^5$	$0.15663249 * 10^5$	0.13944219	
1.971469		$0.43176681 * 10^{15}$	$0.15412547 * 10^{10}$	0.13943256	6523.7912

Table 6. $c_1 = c_2 = 1, \varepsilon = 1$

The CPU (Central Processing Unit) Time is measured in seconds.

RADAU5				
T	h	$u(x_0), x_0 = 0$	$u(x_1), x_1 = h$	$u(x_N), x_N = 1$
0.74	$\frac{1}{3}.10^{-3}$	$.23375982 * 10^3$	$.23371089 * 10^3$	$.50827897 * 10$
0.7451917		$.35872564 * 10^{18}$	$.44785251 * 10^7$	$.53080172 * 10$

Table 7. $c_1 = 1, c_2 = 0, \varepsilon = 1$.

Acknowledgements. The authors are supported by Bulgarian Ministry of Science and Education under Grant MM 524/95.

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Received: 15.04.1999