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A nonlinear weakly singular Volterra integro-differential equation arising from a reaction-diffusion study in a small cell

Jennifer A. DIXON
Oxford University Computing Laboratory, 8-11 Keble Road, Oxford OX1 3QD, United Kingdom

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Abstract: A simple product integration scheme is proposed to solve a nonlinear Volterra integro-differential equation with a weakly singular kernel and a non-smooth solution. A discrete Gronwall inequality is derived and then employed to prove convergence of the numerical method. Numerical results are given which support the theoretical results.

Keywords: Vollerra integro-differential equation, weakly singular kernel, discrete Gronwall inequality, convergence.

1. Introduction

The following diffusion equation models a simple reversible reaction within a small cell:

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t), \qquad 0<x<1, \quad t>0, \tag{1.1a}$$

$$\frac{\partial u}{\partial x}(0,\ t)=0, \quad t>0, \tag{1.1b}$$

$$\frac{\partial u}{\partial x}(1,t)=m\frac{d\theta}{dt}(t)=\frac{Em}{1+L}\{L\theta(t)-(1-\theta(t))u(1,\ t)\} \quad t>0, \tag{1.1c}$$

$$u(x,0)=1, \quad 0<x<1, \tag{1.1d}$$

$$\theta(0)=0, \tag{1.1e}$$

where

$$m\theta(t)+\int_0^1 u(x,\ t)\ \mathrm{d}x=1, \quad t>0, \tag{1.1f}$$

and E, L, m are given constants.

The problem involves a reaction between two reactants X and Y in a cell to produce a complex XY. The species Y is immobilized on a side wall and X is dissolved in solution. The reaction takes place only on the side wall.

At time $t = 0$ a solution of X is introduced to the cell, then as the reaction at the wall proceeds, an X concentration gradient develops, and X diffuses to the wall until equilibrium results. The interest is in predicting the X concentration profile and the concentration of the complex XY as functions of time. In the above model the non-dimensionalized variables $u(x,t)$ and $\theta(t)$ represent the X and XY concentrations, respectively; the constants E, L, m involve the cell width, the initial concentration of Y, the initial concentration of X at the reaction side wall, and the diffusion coefficient of X.

Further discussion of this problem may be found in [6].

By taking the Laplace transform of equation (1.1a), using the initial condition (1.1d), and inverting using the Convolution Theorem, it may be shown that $u(1,t)$ is given by

$$u(1,\ t) = 1 - m\int_0^t k(t-s)\frac{\mathrm{d}\theta}{\mathrm{d}s}(s)\ \mathrm{d}s, \tag{1.2}$$

where the kernel $k(t)$ is given by

$$k(t) = (\pi t)^{-1/2}\left(1 + 2\sum_{n=1}^{\infty} \exp\left(-\frac{n^2}{t}\right)\right). \tag{1.3}$$

For details see [6].

Consequently it follows from (1.1c) that $\mathrm{d}\theta/\mathrm{d}t$ satisfies the nonlinear weakly singular Volterra integro-differential equation

$$\frac{\mathrm{d}\theta}{\mathrm{d}t}(t) = -\frac{E}{1+L}\left\{L\theta(t) - (1-\theta(t))\left(1 - m\int_0^t k(t-s)\frac{\mathrm{d}\theta}{\mathrm{d}s}(s)\mathrm{d}s\right)\right\}, \tag{1.4}$$

with $\theta(0) = 0$.

The aim of this paper is to solve equation (1.4) numerically and then to use the numerical values for $\theta(t)$ in equation (1.2) to find $u(1,t)$; once u is known on the boundary $x = 1$ equation (1.1a) may be solved with (1.1b) and (1.1d) to determine u in the interior $0 < x < 1$, $t > 0$. An order one method will be proposed, a convergence result will be presented and numerical results will be given.

2. Asymptotic behaviour near $t = 0$

Consider the nonlinear Volterra integro-differential equation

$$\theta'(t) = C - E\theta(t) - Cm(1-\theta(t))\int_0^t k(t-s)\theta'(s)\ \mathrm{d}s, \quad t > 0, \tag{2.1}$$

$$\theta(0) = 0,$$

where $C = E/(1+L)$,

$$k(t) = (\pi t)^{-1/2}\left(1 + 2\sum_{n=1}^{\infty} \exp\left(-\frac{n^2}{t}\right)\right),$$

and $\theta'(t)$ denotes $\mathrm{d}\theta(t)/\mathrm{d}t$.

For small t, $\exp(-n^2/t) \ll 1$ for all n and $k(t) \simeq (\pi t)^{-1/2}$. Therefore, as $t \downarrow 0$,

$$\theta'(t) = C - Cm\pi^{-1/2}\int_0^t \frac{\theta'(s)}{(t-s)^{1/2}}\mathrm{d}s. \tag{2.2}$$

This is a linear second kind Volterra integral equation for $\theta'(t)$. The solution of (2.2) may be found explicitly and is given by

$$\text{B'(t)} = CE_{1/2}(-Cmt^{1/2}), \tag{2.3}$$

where $E_\beta(z)$ is the Mittag-Leffler function defined for all $\beta > 0$ by

$$E_\beta(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\beta + 1)}.$$

(See, for example, [7].)

Consequently, since $\theta(0) = 0$, as $t \downarrow 0$

$$\theta(t) = Ct - \tfrac{4}{3}C^2 m\pi^{-1/2} t^{3/2} + \mathrm{O}(t^2). \tag{2.4}$$

It follows that $\theta(t)$ possesses a discontinuous second derivative at the left end point of the range of integration and B(t) is smooth on $[\delta, T]$ for any $\delta > 0$.

It is well-known that a discontinuity in one of the derivatives of the solution of a weakly singular Volterra integral equation can result in the loss of high order accuracy in product integration and collocation schemes. This has been observed, for example, by te Riele [9], Brunner and te Riele [2] and Brunner [1]; see also Dixon [3]. As a result, in this paper an order one method will be considered for solving (2.1).

3. The numerical method

The equations to be solved are

$$\theta'(t) = C - E\theta(t) - Cm(1 - \theta(t)) \int_0^t k(t-s)\theta'(s)\ \mathrm{d}s, \quad 0 \leqslant t \leqslant T, \tag{3.1}$$

$$\theta(0) = 0, \qquad C = E/(1 + L),$$

and

$$u(1, t) = 1 - m \int_0^t k(t-s)\theta'(s)\ \mathrm{d}s, \quad 0 \leqslant t \leqslant T, \tag{3.2}$$

with the kernel $k(t)$ defined by

$$k(t) = (\pi t)^{-1/2}\left(1 + 2\sum_{n=1}^{\infty} \exp\left(-\frac{n^2}{t}\right)\right). \tag{3.3}$$

It is first necessary to truncate the infinite series in (3.3). Let k,(t) denote the kernel truncated after l terms, that is,

$$k_l(t) = (\pi t)^{-1/2}\left(1 + 2\sum_{n=1}^{l} \exp\left(-\frac{n^2}{t}\right)\right). \tag{3.4}$$

Given $T, \epsilon > 0$ l is to be chosen so that

$$|k(t) - k_l(t)| < \epsilon, \text{ for all } t \in [0, T]. \tag{3.5}$$

Now

$$|k(t)-k_l(t)| = 2(\pi t)^{-1/2}\sum_{n=l+1}^{\infty}\exp\left(-\frac{n^2}{t}\right) < 2(\pi t)^{-1/2}\int_l^{\infty}\exp\left(-\frac{n^2}{t}\right)\,\mathrm{d}n$$
$$= \left(\frac{2}{\pi}\right)^{1/2}\int_{(2/t)^{1/2}l}^{\infty}\exp\left(-\frac{x^2}{2}\right)\mathrm{d}x = 1-\phi\left((2/t)^{1/2}l\right),$$

where

$$\phi(z) = \frac{1}{(2\pi)^{1/2}}\int_{-z}^{z}\exp\left(-\frac{x^2}{2}\right)\mathrm{d}x = \left(\frac{2}{\pi}\right)^{1/2}\int_0^z\exp\left(-\frac{x^2}{2}\right)\mathrm{d}x$$

is a normal function; tables of $\phi(z)$ may be found, for example, in [10].

It follows that (3.5) is satisfied if l is chosen such that

$$\phi\left((2/T)^{1/2}l\right) > 1-\epsilon. \tag{3.6}$$

The numerical method which will now be proposed for equation (3.1) will be a product Euler-type method.

Let $t_i = i\Delta t$, $i = 0(1)N$, $N\Delta t = T$; θ_i and u_i will denote approximations to $\theta(t_i)$ and $u(1, t_i)$, respectively.

Replacing k(t) by $k_l(t)$ in (3.1)

$$\theta'(t_i) \simeq C - E\theta(t_i) - Cm(1-\theta(t_i))\sum_{j=0}^{i-1}\int_{t_j}^{t_{j+1}}k_l(t_i-s)\theta'(s)\,\mathrm{d}s.$$

For $t\in[t_j, t_{j+1}]$ approximate $\theta(t)$ by the linear Lagrange polynomial

$$\frac{1}{\Delta t}\left[(t-t_j)\theta(t_{j+1}) - (t-t_{j+1})\theta(t_j)\right]. \tag{3.7}$$

Then using the approximation

$$\int_{t_j}^{t_{j+1}}\exp\left(-\frac{n^2}{t_i-s}\right)\frac{1}{(t_i-s)^{1/2}}\,\mathrm{d}s \simeq \exp\left(-\frac{n^2}{t_i-t_j}\right)\int_{t_j}^{t_{j+1}}\frac{\mathrm{d}s}{(t_i-s)^{1/2}}, \tag{3.8}$$

leads to the scheme

$$\theta_0 = 0,$$
$$\frac{\theta_i-\theta_{i-1}}{\Delta t} = C - E\theta_i - Cm\pi^{-1/2}(1-\theta_i)\Delta t\sum_{j=0}^{i-1}\gamma(i-j)\left(\frac{\theta_{j+1}-\theta_j}{\Delta t}\right),\quad i = 1(1)N, \tag{3.9}$$

where the quadrature weights $\gamma(i-j)$ are given by

$$\gamma(i-j) = \frac{1}{\Delta t}\left(1+2\sum_{n=1}^{l}\exp\left(-\frac{n^2}{t_i-t_j}\right)\right)\int_{t_j}^{t_{j+1}}\frac{\mathrm{d}s}{(t_i-s)^{1/2}},$$
$$j = 0(1)i-1,\qquad i = 1(1)N. \tag{3.10}$$

As it stands, this scheme requires the solution of a nonlinear equation at each time step since the right hand side of (3.9) involves a term θ_i^2. This may be avoided by replacing $(1-\theta_i)$ by $(1-\theta_{i-1})$, which is an order one approximation.

On rearranging the scheme for evaluating θ_i, $i = 1(1)N$, becomes

$$\theta_0 = 0,\ \theta_i = \frac{1}{\psi_i}\left(\Delta t + \theta_{i-1} + Cm\pi^{-1/2}(1-\theta_{i-1})\Delta t \sum_{j=1}^{i-1}\left(\gamma(i-j) - \gamma(i-j+1)\right)\theta_j\right),$$
$$i = 1(1)N, \tag{3.11}$$

where

$$\psi_i = 1 + E\Delta t + Cm\pi^{-1/2}\Delta t\gamma(1)(1-\theta_{i-1}),$$

with $\gamma(i-j)$ given by (3.10).

The corresponding discretization of (3.2) is

$$u_0 = 1, \tag{3.12}$$
$$u_i = 1 - m\pi^{-1/2}\sum_{j=0}^{i-1}\gamma(i-j)(\theta_{j+1}-\theta_j), \quad i = 1(1)N.$$

Note that in evaluating θ_i the summation

$$a_i = \gamma(1)\theta_{i-1} - \sum_{j=0}^{i-2}\gamma(i-j)(\theta_{j+1}-\theta_j)$$

has already been found and u_i is then determined by

$$u_i = 1 - m\pi^{-1/2}(\gamma(1)\theta_i - a_i).$$

4. The convergence result

The main result of this paper is the following convergence result for the numerical scheme (3.11), (3.12).

Theorem 4.1. *Let $\theta(t)$ and $u(1,t)$ be the solutions of equations (3.1) and (3.2) respectively. Let $T > 0$ and $\delta > 0$ (with $\delta < T$) be given. Given $\Delta t_{\min} > 0$ take r to be the smallest integer such that $r\Delta t_{\min} > \delta$, and choose $l = l(T)$ so that*

$$|k(t) - k_l(t)| < \hat{C}\Delta t_{\min} \text{ for all } t \in [0, T], \tag{4.1}$$

where $k(t)$, $k_l(t)$ are given respectively by (3.3), (3.4).

Let θ_i, u_i, $i = 0(1)N$, be the solutions of the discretizations (3.11) (3.12). Then for all $\Delta t \geqslant \Delta t_{\min}$ sufficiently small the error $e_i = \theta(t_i) - \theta_i$ satisfies

$$|e_i - e_{i-1}| \leqslant \begin{cases} C_1'\Delta t^{3/2} + O(\Delta t^2), & i = 1(1)r-1, \\ C_2'\Delta t^2 + O(\Delta t^{5/2}), & i = r(1)N, \end{cases} \tag{4.2}$$

and

$$|u(1,t_i) - u_i| \leqslant C_3'\Delta t + O(\Delta t^{3/2}), \quad i = 0(1)N. \tag{4.3}$$

In the above theorem, and throughout this paper, constants C, M, with or without subscripts and/or superscripts, will denote constants which are (possibly) dependent on T but independent of At.

Note that (4.2) implies

$$|e_i| \leqslant C_4'\Delta t + O(\Delta t^{3/2}), \quad i = r(1)N. \tag{4.4}$$

For if

$$|e_i - e_{i-1}| \leqslant b_i,$$

then $||e_i| - |e_{i-1}|| \leqslant b_i$. That is, $-b_i \leqslant |e_i| - |e_{i-1}| \leqslant b_i$, which implies $|e_i| \leqslant \sum_{j=1}^{i} b_j$. Therefore

$$|e_i| \leqslant \begin{cases} r\left(C_1'\Delta t^{3/2} + O(\Delta t^2)\right), & i = 1(1)r-1 \\ r\left(C_1'\Delta t^{3/2} + O(\Delta t^2)\right) + (i-r)\left(C_2'\Delta t^2 + O(\Delta t^{5/2})\right), & i = r(1)N, \end{cases}$$

and, since $i\Delta t \leqslant T$, (4.4) follows.

The proof of Theorem 4.1 will be given in the next section. The presence of the term $(1 - \theta(t))$ multiplying the integral on the right hand side of equation (3.1) means that the usual convergence analysis presented, for example, by McKee [8], is not applicable. However, the convergence analysis will follow the usual steps employed when looking at the convergence of a numerical scheme for solving a Volterra equation. The order of the consistency error will be considered in the remainder of this section and then in the next section, the consistency error will be related to $|e_i - e_{i-1}|$ using a discrete Gronwall inequality (Lemma 5.1). The main new feature in the argument is the necessity in this paper to consider $|e_i - e_{i-1}|$, in place of $|e_i|$.

The consistency error T_i, i = 1(1) N, of the scheme (3.11) is defined to be

$$T_i = \frac{\theta(t_i) - \theta(t_{i-1})}{\Delta t} - C + E\theta(t_l) + Cm\pi^{-1/2}(1 - \theta(t_{i-1}))\Delta t \sum_{j=0}^{i-1} \gamma(i-j)\left\{\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t}\right\}. \tag{4.5}$$

The following lemma investigates the order of consistency.

Lemma 4.1. *Let r and l be chosen as in Theorem 4.1. Then for all* At $\geqslant$ At$_{\min}$ *the consistency error* T_i *defined by* (4.5) *satisfies*

$$|T_i| \leqslant \begin{cases} C_1\Delta t^{1/2} + O(\Delta t), & i = 1(1)r-1, \\ C_2\Delta t + 0(\text{ At*}), & i = r(1)N. \end{cases} \tag{4.6}$$

Proof. Using (3.1) the consistency error T_i may be written as

$$T_i = \frac{\theta(t_i) - \theta(t_{i-1})}{\text{At}} - \theta'(t_i) - Cm(l - \theta(t_i))\sum_{j=0}^{i-1}\int_{t_j}^{t_{j+1}} k(t_i - s)\theta'(s)\,ds + Cm\pi^{-1/2}(1 - \theta(t_{i-1}))\sum_{j=0}^{i-1} y(i-j)\left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\text{At}}\right)$$

Therefore,

$$T_i = \left(\frac{\theta(t_i) - \theta(t_{i-1})}{\Delta t} - \theta'(t_i) \right)$$
$$- Cm(1-\theta(t_{i-1})) \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} k_l(t_i - t_j) \left\{ \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right\} \mathrm{d}s$$
$$+ Cm(1-\theta(t_{i-1})) \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} \{ k_l(t_i - t_j) - k_l(t_i - s) \} \theta'(s) \, \mathrm{d}s$$
$$+ Cm(1-\theta(t_{i-1})) \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} \{ k_l(t_i - s) - k(t_i - s) \} \theta'(s) \, \mathrm{d}s$$
$$+ Cm(\theta(t_i) - \theta(t_{i-1})) \int_0^{t_i} k(t_i - s) \theta'(s) \, \mathrm{d}s. \tag{4.7}$$

Since $\theta(t)$ is smooth on $[\delta, T]$, for $s \in [t_j, t_{j+1}]$, $j = r(1)N-1$,

$$\left| \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right| \leqslant M_1 \Delta t. \tag{4.8}$$

Using the asymptotic expansion (2.4) for small t it follows that for $s \in [t_j, t_{j+1}]$, $j = 0(1)r-1$,

$$\left| \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right| \leqslant M_2 \Delta t^{1/2} + \mathrm{O}(\Delta t) \tag{4.9}$$

Consequently, for $i \geqslant r$,

$$\left| \sum_{j=0}^{r-1} \int_{t_j}^{t_{j+1}} k_l(t_i - t_j) \left\{ \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right\} \mathrm{d}s \right|$$
$$\leqslant \left(M_2 \Delta t^{1/2} + \mathrm{O}(\Delta t) \right) \Delta t \sum_{j=0}^{r-1} k_l(t_i - t_j).$$

But, for $i \geqslant r$,

$$\Delta t \sum_{j=0}^{r-1} k_l(t_i - t_j) = \Delta t \sum_{j=0}^{r-1} \pi^{-1/2} \left(1 + 2 \sum_{n=1}^{l} \exp\left(- \frac{n^2}{t_i - t_j} \right) \right) \frac{1}{(t_i - t_j)^{1/2}}$$
$$\leqslant C^* \Delta t \sum_{j=0}^{r-1} \frac{1}{(t_i - t_j)^{1/2}}$$
$$\leqslant C^* \int_0^{t_r} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} \leqslant C^* \int_0^{t_r} \frac{\mathrm{d}s}{(t_r - s)^{1/2}} = 2C^*(r\Delta t)^{1/2}.$$

Hence, for $i \geqslant r$,

$$\left| \sum_{j=0}^{r-1} \int_{t_j}^{t_{j+1}} k_l(t_i - t_j) \left\{ \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right\} \mathrm{d}s \right| \leqslant \hat{C} \Delta t + \mathrm{O}(\Delta t^{3/2}). \tag{4.10a}$$

For $i \leqslant r-1$,

$$\Delta t \sum_{j=0}^{i-1} k_l(t_i - t_j) \leqslant C^* \Delta t \sum_{j=0}^{i-1} \frac{1}{(t_i - t_j)^{1/2}}$$

$$\leqslant C^* \int_0^{t_i} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} = 2C^* t_i^{1/2} < 2C^*(r\Delta t)^{1/2},$$

and

$$\left| \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} k_l(t_i - t_j) \left\{ \theta'(s) - \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) \right\} \mathrm{d}s \right| \leqslant \hat{C}\Delta t + \mathrm{O}(\Delta t^{3/2}). \tag{4.10b}$$

Since $\theta'(t)$ is continuous on $[0, T]$

$$|\theta(t_i) - \theta(t_{i-1})| \leqslant M_3 \Delta t, \quad i = 1(1)N. \tag{4.11}$$

Also, for $s \in [t_j, t_{j+1}]$,

$$\left| \exp\left(-\frac{n^2}{t_i - t_j} \right) - \exp\left(-\frac{n^2}{t_i - s} \right) \right| \leqslant M_4 \Delta t,$$

so that

$$|k_l(t_i - t_j) - k_l(t_i - s)| \leqslant M_5 \Delta t. \tag{4.12}$$

Using (4.8)–(4.12) and (4.1) in (4.7) the required result may be deduced. □

The consistency error $\hat{T}_i, i = 1(1)N$, of the scheme (3.12) for determining $\{u_i\}_{i=1}^{N}$ is given by

$$\hat{T}_i = u(1, t_i) - 1 + m\pi^{-1/2} \sum_{j=0}^{i-1} \gamma(i-j)(\theta(t_{j+1}) - \theta(t_j)).$$

Lemma 4.2. *Under the same hypotheses as Lemma 4.1 the consistency error* $\hat{T}_i$ *satisfies*

$$|\hat{T}_i| \leqslant \tilde{C}\Delta t + \mathrm{O}(\Delta t^2), \quad i = 1(1)N. \tag{4.13}$$

Proof. The consistency error $\hat{T}_i$ may be rewritten as

$$\hat{T}_i = m \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} k_l(t_i - t_j) \left\{ \left(\frac{\theta(t_{j+1}) - \theta(t_j)}{\Delta t} \right) - \theta'(s) \right\} \mathrm{d}s$$

$$+ m \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} (k_l(t_i - t_j) - k_l(t_i - s)) \theta'(s) \, \mathrm{d}s$$

$$+ m \sum_{j=0}^{i-1} \int_{t_j}^{t_{j+1}} (k_l(t_i - s) - k(t_i - s)) \theta'(s) \, \mathrm{d}s.$$

Using (4.1), (4.8), (4.10) and (4.12) the bound (4.13) follows. □

5. The proof of convergence

In this section the proof of Theorem 4.1 will be presented. First some preliminary results are required.

The consistency error T_i defined by (4.5) will be related to the error $|e_i - e_{i-1}|$ using the following discrete Gronwall inequality.

Lemma 5.1. *Let x_i, $i = 0(1)N$, be a sequence of non-negative real numbers. If*

$$x_i \leqslant \phi_i + M\Delta t^{1-\alpha} \sum_{j=0}^{i-1} \frac{x_j}{(i-j)^{\alpha}}, \quad i = 0(1)N, \tag{5.1}$$

where $\alpha \in (0, 1)$, $M > 0$ is independent of At, and

$$0 \leqslant \phi_i \leqslant \begin{cases} \delta_1, & i = 0(1)r-1, \\ \delta_2, & i = r(1)N, \end{cases} \tag{5.2}$$

for some integer r, independent of At, then

$$x_i \leqslant \begin{cases} \delta_1\left(1 + \Delta t^{1-\alpha} M\Gamma(1-\alpha) r \sum_{n=0}^{\infty} \frac{\left(M\Gamma(1-\alpha)(i\Delta t)^{1-\alpha}\right)^n}{\Gamma((n+1)(1-\alpha))}\right), \quad i = 1(1)r-1, & (5.3a) \\ \delta_2\left(1 + E_{1-\alpha}\left(M\Gamma(1-\alpha)(i\Delta t)^{1-\alpha}\right)\right) & \\ \quad + \delta_1 \Delta t^{1-\alpha} M\Gamma(1-\alpha) r \sum_{n=0}^{\infty} \frac{\left(M\Gamma(1-\alpha)(r\Delta t)^{1-\alpha}\right)^n}{\Gamma((n+1)(1-\alpha))}, \quad i = r(1)N. & (5.3b) \end{cases}$$

Corollary 5.1. *If x_i, $i = 0(1)N$, satisfies (5.1), (5.2) and $N\Delta t \leqslant T$, then there exists positive constants $C_1 = C_1(T)$, $C_2 = C_2(T)$, independent of At, such that*

$$x_i \leqslant \begin{cases} \delta_1\left(1 + C_1 \Delta t^{1-\alpha}\right), & i = 0(1)r-1, \quad (5.4a) \\ \delta_2 C_2 + \delta_1 C_1 \Delta t^{1-\alpha}, & i = r(1)N. \quad (5.4b) \end{cases}$$

Proof. From the results of Dixon and McKee [4] (see also [5]) it follows that (5.1) implies x_i, $i = 0(1)N$, satisfies

$$x_i \leqslant \phi_i + \sum_{n=1}^{\infty} \Delta t \sum_{j=0}^{i-1} k_{ij}^{(n)} \phi_j, \tag{5.5}$$

where

$$k_{ij}^{(1)} = k_{ij} = M(\Delta t(i-j))^{-\alpha} \quad \text{and} \quad k_{ij}^{(n)} = \Delta t \sum_{l=j+1}^{i-1} k_{il} k_{lj}^{(n-1)}, \quad n \geqslant 2. \tag{5.6}$$

Moreover, Dixon and McKee show that with k_{ij} defined by (5.6), $k_{ij}^{(n)}$ satisfies

$$k_{ij}^{(n)} \leqslant \frac{(M\Gamma(1-\alpha))^n}{\Gamma(n(1-\alpha))} (\Delta t(i-j))^{(n-1)-n\alpha}, \quad n \geqslant 1, \tag{5.7}$$

and that

$$\sum_{n=0}^{\infty} \Delta t \sum_{j=0}^{i-1} k_{ij}^{(n)} \leqslant E_{1-\alpha}\left(M\Gamma(1-\alpha)(i\Delta t)^{1-\alpha}\right), \quad i = 0(1)N. \tag{5.8}$$

Using (5.7) in (5.5), for $i = 0(1)r-1$,

$$x_i \leqslant \delta_1 \left\{1 + \sum_{n=1}^{\infty} \Delta t \sum_{j=0}^{i-1} \frac{(M\Gamma(1-\alpha))^n}{\Gamma(n(1-\alpha))} (\Delta t(i-j))^{(n-1)-n\alpha}\right\}$$

$$\leqslant \delta_1 \left\{1 + \Delta t^{1-\alpha} \sum_{n=1}^{\infty} \frac{(M\Gamma(1-\alpha))^n}{\Gamma(n(1-\alpha))} \sum_{j=0}^{i-1} (\Delta t(i-j))^{(n-1)(1-\alpha)}\right\}$$

$$\leqslant \delta_1 \left\{1 + r\Delta t^{1-\alpha} \sum_{n=1}^{\infty} \frac{(M\Gamma(1-\alpha))^n}{\Gamma(n(1-\alpha))} (i\Delta t)^{(n-1)(1-\alpha)}\right\},$$

which yields (5.3a).

For $i = r(1)N$

$$x_i \leqslant \delta_2 + \delta_1 \sum_{n=1}^{\infty} \Delta t \sum_{j=0}^{r-1} k_{ij}^{(n)} + \delta_2 \sum_{n=1}^{\infty} \Delta t \sum_{j=r}^{i-1} k_{ij}^{(n)}.$$

Using (5.8) to bound the last term on the right and employing the same arguments as above to bound the second term on the right, (5.3b) follows immediately. □

To deduce the corollary, note that $i\Delta t \leqslant T$, $i = 0(1)N$, and use the fact that the series

$$\sum_{n=0}^{\infty} \frac{\left(M\Gamma(1-\alpha)T^{1-\alpha}\right)^n}{\Gamma((n+1)(1-\alpha))}$$

is convergent for all T and is thus bounded for all T.

A bound on the quadrature weights will be required in the convergence analysis. A bound is given by the following lemma.

Lemma 5.2. *The quadrature weights $\gamma(i-j)$ defined by (3.10) satisfy*

$$0 \leqslant \gamma(i-j+1) \leqslant \begin{cases} M(\Delta t(i-j)) & 0(1)i-1, \\ M\Delta t^{-1/2}, & j = i. \end{cases} \tag{5.9}$$

Moreover,

$$\gamma(i-j) > \gamma(i-j+1), \quad j = 0(1)i-1. \tag{5.10}$$

Proof. For $j \leqslant i-1$,

$$0 \leqslant \gamma(i-j) = \frac{1}{\Delta t}\left\{1 + 2\sum_{n=1}^{l} \exp\left(-\frac{n^2}{t_i - t_j}\right)\right\} \int_{t_j}^{t_{j+1}} \frac{\mathrm{d}s}{(t_i - s)^{1/2}}$$

$$\leqslant \frac{\hat{C}(T)}{\Delta t} \int_{t_j}^{t_{j+1}} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} = \hat{C}(T)(\Delta t(i-j))^{-1/2} \int_0^1 \frac{\mathrm{d}p}{(1 - p/(i-j))^{1/2}}$$

$$\leqslant M(\Delta t(i-j))^{-1/2}.$$

Hence, for $j \leqslant i$,

$$\gamma(i-j+1) \leqslant M(\Delta t(i-j+1))^{-1/2}.$$

For $j \leqslant i-1, (i-j+1)^{-1/2} \leqslant (i-j)^{-1/2}$, and (5.9) is immediate. For all i,

$$i^{1/2} - (i-1)^{1/2} > (i+1)^{1/2} - i^{1/2},$$

and for all positive integers n and At sufficiently small

$$\left(i^{1/2} - (i-1)^{1/2}\right) \exp\left\{\frac{-n^2}{i\Delta t}\right\} > \left((i+1)^{1/2} - i^{1/2}\right) \exp\left\{\frac{-n^2}{(i+1)\Delta t}\right\},$$

$$i = 1(1)N-1, \qquad Nh = T.$$

It may be deduced that

$$\gamma(i) > \gamma(i+1), \quad i = 1(1)N-1,$$

and (5.10) follows. • I

The following bound on θ_i will be employed in the proof of Theorem 4.1.

Lemma 5.3. *The sequence* $\{\theta_i\}_{i=0}^{N}$ *defined by (3.11) satisfies*

$$0 < \theta_i < 1, \ i = 1, 2, 3, \ldots\ldots \tag{5.11}$$

Proof. The proof uses an inductive argument.

Since $\theta_0 = 0$ it is clear from (3.11) that (5.11) is satisfied for $i = 1$.

Assume inductively that (5.11) is satisfied for $i = 1, 2, \ldots, k-1$. It then follows using (5.10) that $\theta_k > 0$ and, from (3.11), $\theta_k < 1$ provided

$$\theta_{k-1} + C\Delta t + Cm\pi^{-1/2}(1-\theta_{k-1})\Delta t \sum_{j=1}^{k-l} (\gamma(k-j) - \gamma(k-j+1))\theta_j$$

$$< 1 + E\Delta t + Cm\pi^{-1/2}\Delta t\gamma(1)(1-\theta_{k-1}). \tag{5.12}$$

By hypothesis $\theta_{k-1} < 1$ and, since $L > 0$, $C < E$. Moreover, since by assumption $0 < \theta_j < 1$, $j = 1(1)k-1$,

$$\sum_{j=1}^{k-l} (\gamma(k-j) - \gamma(k-j+1))\theta_j < \sum_{j=1}^{k-1} (\gamma(k-j) - \gamma(k-j+1)) = \gamma(1).$$

Thus (5.12) holds and the inductive step is complete. □

Using Lemmas 5.1-5.3 the proof of Theorem 4.1 is now given.

Proof of Theorem 4.1. From (3.11) and (4.5) the error $e_i = \theta(t_i) - \theta_i$ satisfies

$$\begin{aligned} e_i - e_{i-1} = {} & -Ee_i\Delta t - Cm\pi^{-1/2}\Delta t \sum_{j=0}^{i-1} \gamma(i-j)(e_{j+1} - e_j) \\ & + Cm\pi^{-1/2}\Delta t \sum_{j=0}^{i-1} \gamma(i-j)\left\{\theta(t_{i-1})\left(\theta(t_{j+1}) - \theta(t_j)\right) - \theta_{i-1}(\theta_{j+1} - \theta_j)\right\} \\ & + \Delta t T_i \\ = {} & -Ee_i\Delta t - Cm\pi^{-1/2}\Delta t(1 - \theta_{i-1}) \sum_{j=0}^{i-1} \gamma(i-j)(e_{j+1} - e_j) \\ & + Cm\pi^{-1/2}\Delta t e_{i-1} \sum_{j=0}^{i-1} \gamma(i-j)\left(\theta(t_{j+1}) - \theta(t_j)\right) + \Delta t T_i. \end{aligned}$$

Set $z_i = e_i - e_{i-1}$, $i = 1(1)N$, $z_0 = 0$, and observe that

$$e_i = \sum_{j=0} z_j.$$

Then z_i, $i = 0(1)N$, satisfies

$$\begin{aligned} z_i = {} & -E\Delta t \sum_{j=0}^{i} z_j - Cm\pi^{-1/2}\Delta t(1 - \theta_{i-1}) \sum_{j=0}^{i-1} \gamma(i-j) z_{j+1} \\ & + Cm\pi^{-1/2}\Delta t \sum_{k=0}^{i-1} z_k \sum_{j=0}^{i-1} \gamma(i-j)\Delta t\theta'(\eta_j) + \Delta t T_i, \end{aligned}$$

for some $\eta_j \in (t_j, t_{j+1})$.

From Lemma 5.3

$$0 < \theta_j < 1, \quad j = 0, 1, \ldots.$$

Also

$$\begin{aligned} \Delta t \sum_{j=0}^{i-1} \gamma(i-j) &= \sum_{j=0}^{i-1} \left\{1 + 2\sum_{n=1}^{l} \exp\left(-\frac{n^2}{t_i - t_j}\right)\right\} \int_{t_j}^{t_{j+1}} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} \\ &\leqslant C^* \int_0^{t_i} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} = 2C^* t_i^{1/2}. \end{aligned} \tag{5.13}$$

Therefore,

$$|z_i| \leqslant E\Delta t \sum_{j=0}^{i} |z_j| + Cm\pi^{-1/2}\Delta t \sum_{j=1}^{i} \gamma(i-j+1)|z_j| + M_1\Delta t \sum_{j=0}^{i-1} |z_j| + \Delta t|T_i|,$$

where $M_1 = 2C^* Cm\pi^{-1/2}T^{1/2} \max_{0 \leqslant t \leqslant T} |\theta'(t)|$.

Invoking Lemma 5.2 gives

$$\begin{aligned} & (1 - E\Delta t - MCm\pi^{-1/2}\Delta t^{1/2})|z_i| \\ & \quad \leqslant (M_1 + E)\Delta t \sum_{j=0}^{i-1} |z_j| + MCm\pi^{-1/2}\Delta t^{1/2} \sum_{j=1}^{i-1} \frac{|z_j|}{(i-j)^{1/2}} + \Delta t|T_i|. \end{aligned}$$

But

$$At \sum_{j=O}^{i-l} | z, | = \Delta t^{1/2} \sum_{j=O}^{i-1} \frac{|z_j|}{(i - j)^{1/2}} ((i-j)\Delta t)^{1/2} \leqslant \quad T^{1/2}\Delta t^{1/2} \sum_{j=0}^{i-1} \frac{|z_j|}{(i-j)^{1/2}}$$

It follows that provided At $\geqslant$ At,, is chosen so that

$$E\Delta t - MCm\pi^{-1/2}\Delta t^{1/2} < 1,$$

$|z_i|, i = 0(1)N$, satisfies the inequality

$$|z_i| \leqslant C'\Delta t\, |T_i| + M'\Delta t^{1/2} \sum_{j=O}^{i-1} \frac{|z_j|}{(i-j)^{1/2}}, \quad i = 0(1)N,$$

for some C’, M’ > 0.

By Lemma 4.1

$$|T_i| \leqslant \begin{cases} C_1\Delta t^{1/2} + O(\Delta t), & i = 1(1)r - 1, \\ C_2\Delta t + 0(\text{ At'}), & i = r(1)N, \end{cases}$$

(with $T_0 = 0$).

Employing Corollary 5.1 with $\alpha = \frac{1}{2}$ yields

$$|z_i| \leqslant \begin{cases} C_1'\Delta t^{3/2} + O(\Delta t^2), & i = 1(1)r - 1, \\ C_2'\Delta t^2 + O(\Delta t^{5/2}), & i = r(1)N. \end{cases}$$

This proves (4.2).

The error $\hat{e}_i = u(1, t_i) - u_i$, $i = 0(1)N$, satisfies

$$\hat{e}_i = m\pi^{-1/2} \sum_{j=0}^{i-1} \gamma(i-j)(e_{j+1} - e,) + \hat{T}_i,$$

with $\hat{e}_0 = 0$.

By (5.13), for $i = 1(1)r - 2$,

$$\sum_{j=0}^{i-1} \gamma(i-j) < \frac{2C^*}{\Delta t} t_i^{1/2} < \frac{2C^* r^{1/2}}{\Delta t^{1/2}}.$$

Using (4.2) and Lemma 4.2 the bound (4.3) is now immediate for $i = 1(1)r - 2$.

For $i = r - 1(1)N$,

$$|\hat{e}_i| \leqslant m\pi^{-1/2} \left\{ \sum_{j=O}^{r-2} \gamma(i-j)|e_{j+1} - e_j| + \sum_{j=r-1}^{i} \gamma(i-j)\,|e_{j+1} - e_j| \right\} + |\hat{T}_i|,$$

and

$$\sum_{j=0}^{r-2} \gamma(i-j) < \frac{C^*}{\Delta t} \sum_{j=0}^{r-2} \int_{t_j}^{t_{j+1}} \frac{\mathrm{d}s}{(t_i - s)^{1/2}} \leqslant \frac{\bar{C} r^{1/2}}{\Delta t^{1/2}}.$$

From (5.13), (4.2) and Lemma 4.2 the bound (4.3) follows for $i = r - 1(1)N$. The theorem is thus proved. ❑

From Theorem 4.1 it follows (by recalling (4.4)) that away from the origin the discretizations (3.11), (3.12) for evaluating θ_i, u_i, respectively, are convergent of order one.

6. Numerical results

Let $\tilde{\theta}_1, \tilde{\theta}_2, \tilde{\theta}_4$ and $\tilde{u}_1, \tilde{u}_2, \tilde{u}_4$ denote the computed values of $\theta(t)$ and $u(1, t)$, at a given fixed point t, obtained by steplengths At, $2\Delta t, 4\Delta t$, respectively. Suppose that the cumulative errors for the θ- and u-schemes, defined by (3.11), (3.12), are proportional to $M_1\Delta t^{q1}$ and $M_2\Delta t^{q2}$, respectively, where M_i, q_i, i = 1, 2, are unknown constants.

Then

$$\theta(t)-\tilde{\theta}_1 = M_1\Delta t^{q_1}, \qquad \theta(t)-\tilde{\theta}_2 = M_1(2\Delta t)^{q_1}, \qquad \theta(t)-\tilde{\theta}_4 = M_1(4\Delta t)^{q_1},$$

and

$$u(1, t) - \tilde{u}_1 = M_2\Delta t^{q_2}, \qquad u(1, t) - \tilde{u}_2 = M_2(2\Delta t)^{q_2}, \qquad u(1, t) - \tilde{u}_4 = M_2(4\Delta t)^{q_2}.$$

(Note that in general equality does not hold but for simplicity is assumed here: the argument used is intended to be a heuristic one.)

Hence

$$\left(\theta(t) - \tilde{\theta}_1\right)/\left(\theta(t) - \tilde{\theta}_2\right) = \left(\theta(t) - \tilde{\theta}_2\right)/\left(\theta(t) - \tilde{\theta}_4\right) = 1/2^{q_1}.$$

Solving for $\theta(t)$ gives the Aitken extrapolation formula

$$\theta(t) = \tilde{\theta}_1 - \left(\tilde{\theta}_1 - \tilde{\theta}_2\right)^2/\left(\tilde{\theta}_1 - 2\tilde{\theta}_2 + \tilde{\theta}_4\right), \tag{6.1}$$

and similarly

$$u(1, t) = \tilde{u}_1 - \left(\tilde{u}_1 - \tilde{u}_2\right)^2/\left(\tilde{u}_1 - 2\tilde{u}_2 + \tilde{u}_4\right). \tag{6.2}$$

The parameters

$$x_1 = \left(\tilde{\theta}_4 - \tilde{\theta}_2\right)/\left(\tilde{\theta}_2 - \tilde{\theta}_1\right), \qquad x_2 = \left(\tilde{u}_4 - \tilde{u}_2\right)/\left(\tilde{u}_2 - \tilde{u}_1\right), \tag{6.3}$$

which have theoretical values of 2^{q_1}, 2^{q_2}, respectively, will be used to verify the rates of convergence obtained in Theorem 4.1.

Consider now some numerical results. The method was implemented with various values assigned to the constants E, L, m, within the range of values of practical interest for the problem (1.1); details of the constants E, L, m and their range of values are given in [6]. Results are presented in Table 1 for E = 100, L = 0.01, m = 1.0 with stepsizes At = 0.01, 0.02, and 0.04 up to T = 2.4. For T = 0.4, 1.0, 2.4 l was chosen to be l = 3, 4, 7 respectively. This ensures that ϵ in (3.5) is less than 10-s. Figure 1 shows 8(t) and u(1, t) over [0, 2.4] with At = 0.01, I = 7.

The expected values of x_1, x_2 were $x_1 = x_2 = 2$. Estimates of x_1, x_2 obtained using (6.3) agree closely with this expected value, confirming that convergence of the θ- and u-schemes is of order one.

As $t \to \infty$ equilibrium results. Let $u(1, t) \to \hat{u}$ and $\theta(t) \to \hat{\theta}$ as $t \to \infty$. From (1.1c) and (1.1f) $\hat{\theta}$ and $\hat{u}$ satisfy

$$L\hat{\theta} = (1 - \hat{\theta})\hat{u}, \qquad m\hat{\theta} = 1 - \hat{u}. \tag{6.4a, b}$$

Table 1
$E = 100$, $L = 0.01$, $m = 1.0$

At	θ_i	A	u_i	A
(t_i = 0.4, l = 3)				
0.01	*0.6523*		*0.0586*	
		0.0174		*−0.0153*
0.02	*0.6349*		*0.0739*	
		0.0314		*−0.0272*
0.04	*0.6035*		0.1011	
Extrapolated values:	0.6739		0.0389	
(t, = 1.0, l = 4)				
0.01	0.8607		0.0805	
		0.0117		− 0.0042
0.02	0.8490		0.0847	
		0.0226		− 0.0102
0.04	0.8264		0.0949	
Extrapolated values:	0.8613		0.0776	
(t, = 2.4, I = 7)				
0.01	0.9038		0.0943	
		0.0013		0.0005
0.02	0.9025		0.0938	
		0.0035		0.0008
0.04	0.8990		0.0930	
Extrapolated values:	0.9046		0.0951	

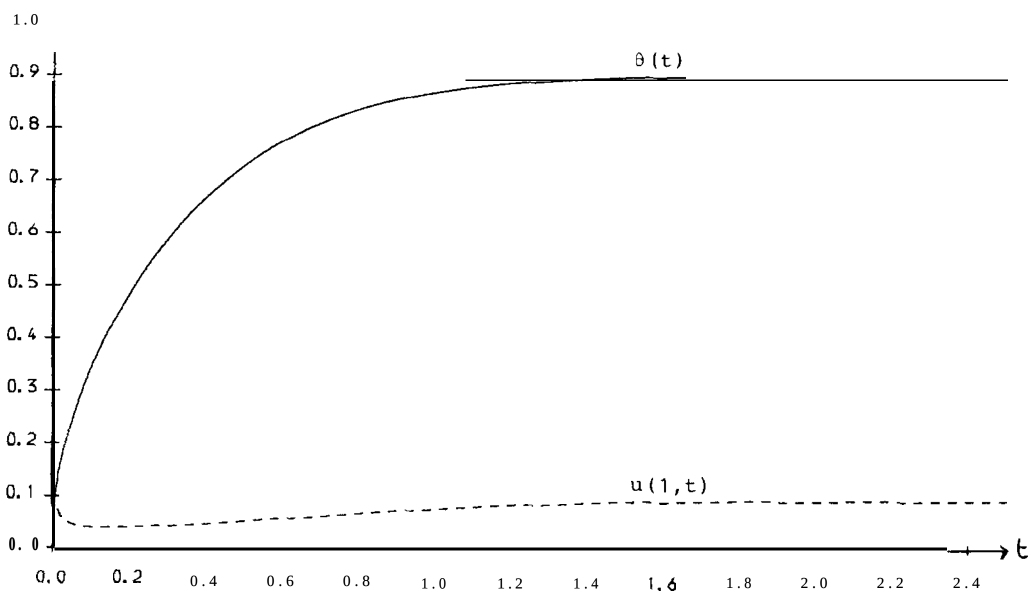

Fig. 1. $E = 100$, $L = 0.01$, $m = 1.0$.

Note that $\hat{\theta}, \hat{u}$ are independent of E.

Equations (6.4a), (6.4b) may be solved for $\hat{\theta}, \hat{u}$. In the case $L = 0.01$, $m = 1.0$ $(E = 100)$ they yield

$$\hat{\theta} = 0.9049, \qquad \hat{u} = 0.0951$$

which may be compared with the extrapolated values as t increases.

7. Concluding remarks

An order one explicit scheme has been used to solve the nonlinear Volterra integro-differential equation (1.4) and hence to find the solution of equation (1.1) on the boundary x = 1. It is then straightforward to solve (1.1) in the interior $0 < x < 1$, $t > 0$ using, for example, the simple implicit method. Numerical results are presented in [6].

A discrete Gronwall inequality has been presented which has been designed to exploit the fact that near the origin the scheme for solving (1.4) is only consistent of order $\Delta t^{1/2}$ but away from the origin is consistent of order At. This Gronwall inequality has been employed to prove convergence of order one, and this is confirmed by the results of numerical experiments.

It is possible using similar, but more complex analysis, to develop product integration or polynomial collocation schemes for the integro-differential equation (1.4) which would be of a higher order if the solution of (1.4) were smooth on [0, T]. However, the non-smoothness of the solution near the left end point of the range of integration means that such a scheme will still only be consistent of order $\Delta t^{1/2}$ near the origin, which would again lead to convergence of only order one.

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