

An Explicit Third-Order Numerical Method For Size-Structured Population Equations

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Abstract

A numerical method incorporating a combination of a difference scheme and several uniform and nonuniform quadrature rules is presented. The method is designed to solve size-structured population equations with linear growth rate and nonlinear fertility and mortality rates. A detailed analysis of the global discretization error is carried out. An example whose exact solutions are known have been solved numerically using a computer implementation of the proposed method. The computations show that the global error is of third order as predicted by the theory.

Keywords: *structured population dynamics, error analysis, quadratures, difference schemes*

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1 Introduction

In this paper we describe a new explicit numerical method of third order for solving size-structured equations of the form

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial g(x)u}{\partial x} &= -\mu(x, P(t))u(x, t), t > 0, x > 0, \\ g(0)u(0, t) &= \int_0^X \beta(x, P(t))u(x, t)dx \\ u(x, 0) &= u_0(x), \end{aligned} \tag{1.1}$$

where

$$P(t) = \int_0^X u(x, t)dx.$$

Problem (1.1) is typical for structured population dynamics, where $u(x, t)$ is a density function representing the population distribution with regard to the structuring variable x . μ and β are the mortality rate and birth function respectively. g is the so called growth rate:

$$\frac{dx}{dt} = g(x).$$

If $g \equiv 1$, this is the so called *age-structured problem*, [10, 17].

The structuring variable x is formally named "size" but in reality it can have the physical meaning of age, size, mass, maturity level, etc.

The method is designed to find a numerical solution to (1.1) in a rectangle $[0, X_1] \times [0, T]$, where $X_1 \geq X$. It is presumed that $\beta(x, P) \geq 0, \mu(x, P) \geq 0, x \in [0, X_1], P \in [0, \infty]$ and that $\frac{\partial \beta}{\partial P}$ and $\frac{\partial \mu}{\partial P}$ are continuous and bounded on $[0, X_1] \times [0, \infty)$. For the method to work and have the desired $O(h^3)$ global discretization error it is necessary that the solution and the above functions have bounded derivatives up to the fourth order on a bounded set (see Theorem 3.1, section 3.5). We also assume that

$$g(x) \neq 0, x \in [0, X_1], \tag{1.2}$$

and that

$$g'(x) + \mu(x, P) \geq 0, x \in [0, X_1], P \in [0, \infty). \tag{1.3}$$

An abundance of papers on numerical schemes for structured equations exists in the literature, but they are designed mainly for age-dependent models. Some of the papers utilize the finite element approach, first used for this type of problem in [4]. The existing numerical methods in the literature can be classified with respect to the order of the global error and to the type of equations they apply to. In [5], [12] are proposed numerical methods for the linear age-structured equation, i.e. with linear with respect to $u(x, t)$ vital functions μ and β : $\mu = \mu(a), \beta = \beta(a)$. The nonlinear age-structured model (with $\mu = \mu(a, P), \beta = \beta(a, P)$) was treated in several papers as follows. Methods with global approximation error $O(h)$ were proposed in [7], [8], [9], [13], [14] [15]

and in the beginning of the 90's. A significantly more accurate method was proposed by Milner and Rabbio, [16]. Theirs is a method of fourth order for the linear case and of second order for the nonlinear case. The idea is based on the observation that the linear equation can be treated as an ODE along the characteristic curves and this idea was implemented using a Runge-Kutta procedure.

A generalization of this paper followed soon in the work by Abia and Lopez-Marcos [1] in which implicit schemes utilizing Runge-Kutta modifications are formulated for the nonlinear case. The schemes are shown to have high order of convergence, but their application is expensive because of the implicitness.

Numerical methods for the linear size-structured equations were proposed in [2] and [11], while the nonlinear equations were considered in [3]. Ito's method is of second order. The methods in [2] and [3] are further generalizations of the methods in [16] for the size-structured case. For the nonlinear equation this generalization naturally is of second order, while for the linear case the order is determined by the one of the employed Runge-Kutta scheme. The last method is proved to work for equations with a nonlinear growth function g and, at present, is unique in this respect.

To the author's best knowledge, no explicit (and therefore cheap) method of order higher than two exists for equations (1.1). It is the purpose of this paper to present such a method. Our method is based on the idea to combine the already widely explored solution on the characteristics, on which all the above mentioned methods are based, with a discretization of an equation for $P(t)$, obtained by integrating (1.1). Using this equation, we calculate an approximation for $P(t)$ *first* and after that we find approximations to the solution $u(x, t)$. Calculating $P(t)$ again by using the approximate values of u will, in general, improve the accuracy of the approximation. The global discretization error of the method proposed in this paper is of third order.

The paper is organized as follows. Section 2 is devoted to some preliminary theoretical issues, such as derivation of the integral equation for P , summary of the quadratures used in the method, etc. Section 3 is a presentation of the method itself, consisting of the generation and approximation of the grid, the discretization formulae and their order of local approximation, and a detailed analysis of the global error. The final part of section 3 is devoted to the construction of $O(h^3)$ approximations to the solution in the initial time layers. Section 4 contains results from a computer implementation of the method.

2 Solving along characteristics

The equation

$$\begin{aligned} \frac{dx}{dt} &= g(x), \\ x(t_0) &= x_0 \end{aligned} \tag{2.1}$$

defines the *characteristic curve* starting at the point (x_0, t_0) . Let $\chi(t; x_0, t_0)$, $x_0 \geq 0, t_0 \geq 0, t \geq 0$ denote the solution of (2.1). On the characteristic curves problem (1.1) has the form

$$\frac{d}{dt}(u(\chi(t; x_0, t_0), t)) = -m(\chi(t; x_0, t_0), P(t)) u(\chi(t; x_0, t_0), t),$$

where $m(x, P) = g'(x) + \mu(x, P)$.

Solving the above equation, we see that if (x_i, t_j) and (x_p, t_q) lie on the same characteristic curve, i.e. $x_i = \chi(t_j; x_p, t_q)$, then

$$u(x_i, t_j) = u(x_p, t_q) e^{-\int_{t_q}^{t_j} m(\chi(\tau; x_p, t_q), P(\tau)) d\tau}. \quad (2.2)$$

2.1 The equation for $P(t)$

Let us integrate (1.1) from 0 to X . We obtain the following equation for P ,

$$\frac{dP}{dt} = -g(X)u(X, t) + \int_0^X [\beta(x, P) - \mu(x, P)]u(x, t) dx \quad (2.3)$$

with initial value

$$P(0) = \int_0^X u_0(x) dx.$$

Let us integrate (2.3) from t_α to t_ω for some given t_α and t_ω . We get

$$P(t_\omega) = P(t_\alpha) - g(X) \int_{t_\alpha}^{t_\omega} u(X, \tau) d\tau + \int_{t_\alpha}^{t_\omega} \int_0^X [\beta(x, P(\tau)) - \mu(x, P(\tau))] u(x, \tau) dx d\tau \quad (2.4)$$

Denote

$$I(t) = -g(X)u(X, t) + \int_0^X [\beta(s, P(t)) - \mu(s, P(t))] u(s, t) ds.$$

Then (2.4) can be written as

$$P(t_\omega) = P(t_\alpha) + \int_{t_\alpha}^{t_\omega} I(\tau) d\tau. \quad (2.5)$$

3 Quadrature rules

Because of the presence of P , obviously each numerical method for this special type of equations should incorporate quadrature rules.

In what follows, h denotes the discretization step.

3.1 Uniform rules

We use several Newton-Cotes quadrature rules of closed and open type, of different order of discretization, namely:

A) *Trapezoidal rule*,

$$Trap[f] = \frac{h}{2}[f(x_0) + f(x_1)] = \int_{x_0}^{x_1} f(x) dx + \frac{1}{12} f^{(2)}(\xi) h^3; \quad (3.1)$$

B) *Open formula of the rectangles,*

$$R_{open}[f] = \frac{3}{2}h[f(x_1) + f(x_2)] = \int_{x_0}^{x_2} f(x)dx - \frac{3}{4}f^{(2)}(\xi)h^3; \quad (3.2)$$

C) *Simpson's rule (closed formula),*

$$Simp[f] = \frac{2h}{6}[f(x_0) + 4f(x_1) + f(x_2)] = \int_{x_0}^{x_2} f(x)dx + \frac{1}{90}f^{(4)}(\xi)h^5; \quad (3.3)$$

D) *A 4-point closed formula,*

$$F_{\frac{3}{8}}[f] = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] = \int_{x_0}^{x_3} f(x)dx + \frac{3}{80}f^{(4)}(\xi)h^5; \quad (3.4)$$

E) *A 5-point open formula*

$$F_{\frac{4}{3}}[f] = \frac{4h}{3}[2f(x_1) - f(x_2) + 2f(x_3)] = \int_{x_0}^{x_4} f(x)dx - \frac{28}{90}f^{(4)}(\xi)h^5 \quad (3.5)$$

In all formulae above ξ is a value located in the integration interval. A glance at the form of the error in each formula shows that the function f must be sufficiently smooth for the quadrature rules to supply the necessary accuracy.

Composite Newton-Cotes quadrature rules are formed by splitting the interval of integration into, say, K subintervals of equal length h and using on each interval a simple quadrature formula. The discretization order of composite quadrature rules is equal to the the one of the participating quadratures minus 1. For example, a composite rule consisting of trapezoidal rules is of order 2 and one consisting of Simpson's rules is of order 4.

3.2 Nonuniform rules

The nodes on the characteristic curves are not uniformly spaced (see next section), so nonuniform quadrature rules are necessary.

Let x_0, \dots, x_n be integration nodes such that $g_0h \leq |x_{i+1} - x_i| \leq g_1h$, where g_0, g_1 are constants independent of h, i . A nonuniform quadrature rule has the form

$$\int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^n \hat{q}_i f(x_i) + R_n \quad (3.6)$$

where

$$R_n \leq \frac{\max_{x \in [x_0, x_n]} |f^{n+1}(x)|}{(n+1)!} (x_n - x_0)^{n+2} = O(h^{n+2}),$$

$$\hat{q}_i = \int_{x_0}^{x_n} \frac{\omega_n(x)}{(x - x_i)\omega'_n(x_i)} dx,$$

and $\omega_n(x) = (x - x_0)\dots(x - x_n)$.

Composite nonuniform quadrature formulae of order $s + 1$ on the interval $[a, b]$ are constructed by applying quadratures of order $s + 2$ on each of the subintervals making up $[a, b]$. Namely, if $x_{ls+j}, l = 0, \dots, M - 1, j = 0, \dots, s$ are the integration nodes, such that $g_0 h \leq |x_{i+1} - x_i| \leq g_1 h$, then, applying simple nonuniform quadratures with accuracy of the order $O(h^{s+2})$ and with coefficients \hat{q}_i^l on each interval $[x_{ls}, x_{(l+1)s}]$, the total error of the composite rule comes out to be of the order $O(h^{s+1})$. In such a case, the coefficients of the composite formula can be written as

$$q_{ps+i} = \begin{cases} \hat{q}_i^p, & \text{if } i = 0, \dots, s - 1, \text{ and } p = 0, \dots, M - 1, \\ \hat{q}_s^p + \hat{q}_0^{p+1}, & i = s \text{ and } p \neq M - 1. \end{cases} \quad (3.7)$$

Finally, $q_{Ms} = \hat{q}_s^M$.

It is easy to establish that

$$q_i \leq Ch$$

where C is a constant independent of h, j . We shall use this estimate in the analysis of the discretization error. For example, C can be esimated as $C = \frac{2(g_1 s)^s}{g_0^s (s-1)!} g_1$. Our method uses values of s not bigger than 4.

3.3 The Numerical Method

3.3.1 Calculating the grid

Let

$$\mathcal{S} = [0, X_1] \times [0, T], X_1 \geq X.$$

We shall calculate a numerical approximation to the solution of (1.1) at certain points of \mathcal{S} . We define these points as the grid $\hat{\mathcal{Z}}$,

$$\hat{\mathcal{Z}} = \{(x_i, t_j), i = 0, \dots, L, j = 0, \dots, N\},$$

where x_i and t_j are defined as follows.

Consider a characteristic curve starting at $x_0 = X, t_0 = 0$. Solving (2.1) for $t < 0$, let $T_l < 0$ be such that $\chi(T_l; X, 0) = 0$. Let $|T_l|/K = h$, where $K = 3M + 4, M$ is an integer and h is the discretization step. Now, let $x_i = \chi(T_l + ih; 0, T_l), i = 0, \dots, K$. Obviously, $x_0 = 0, x_K = X$. Further, let L be such that $x_L = \chi(T_l + Lh; 0, T_l) < X_1 < x_{L+1} = \chi(T_l + (L + 1)h; 0, T_l)$. Further, let N be such that $Nh < T < (N + 1)h$. We shall find numerical approximations to $u(x_i, t_j), i = 0, \dots, L, j = 0, \dots, N$.

It is easy to see that each pair (x_i, t_j) and $(x_{i+1}, t_{j+1}), i = 0, \dots, L - 1, j = 0, \dots, N - 1$ is located on the same characteristic curve. The grid is rectangular (i.e., the grid points are vertices of rectangles), but is not uniform. Because $g(x)$ is continuous and positive on $[0, X]$ and since

$$h = \int_{x_i}^{x_{i+1}} \frac{1}{g(x)} dx,$$

it follows that

$$h \min_{x \in [0, X]} g(x) = hg_0 \leq |x_{i+1} - x_i| \leq hg_1 = h \max_{x \in [0, X]} g(x). \quad (3.8)$$

Recall that the above estimate is necessary to hold in order to apply nonuniform quadrature rules (see the previous section).

3.3.2 Approximating the grid

The grid $\tilde{\mathcal{Z}}$, as defined in the previous section, must be approximated itself. In our case this can be done *before* the calculation of the solution of (1.1). We find numerically a set of points $(y_i, t_j), i = 0, \dots, L, j = 0, \dots, N$, approximating the grid nodes (x_i, t_j) by solving equation (2.1) using a suitable discretization method. In what follows further we assume that $y_i = x_i + O(h^4)$, while t_j are assumed to be exactly known.

Following this procedure, we obtain the *approximate grid*

$$\tilde{\mathcal{Z}} = \{(y_i, t_j), i = 0, \dots, L, j = 0, \dots, N\}.$$

3.3.3 The method

The method is based on successive discretizations of formulae (2.5) and (2.2).

Equation (2.5) is discretized by using quadrature formulae with step h . The time integrals are discretized using a 5 point open Newton-Cotes rule (3.5), thus obtaining explicit formulae. The integrals in s are discretized using a nonuniform composite rule with accuracy $O(h^4)$. The composite rule is constructed as follows. Since the number of points is $K + 1 = 3M + 5$, an open nonuniform rule involving only y_1, y_2, y_3 is used for the first 5 points y_0, y_1, y_2, y_3, y_4 and further, closed 4 point rules are used for each of the set of points $y_{4+3s}, y_{5+3s}, y_{6+3s}, y_{4+3(s+1)}, s = 0, \dots, M - 1$. Each of the 4-point rules have accuracy $O(h^5)$, while the open 5-point rule is of accuracy $O(h^4)$, thus the composite rule is of order $O(h^4)$.

More specifically, assume that the solution $u(x, t)$ is continuous and denote

$$P_{\max} = X \max_{(x,t) \in \mathcal{S}} u(x, t).$$

Obviously P_{\max} is an upper estimate for $P(t)$.

If

$$\frac{\partial^4 u}{\partial t^4} \in C(\mathcal{S}), \frac{\partial^4 \beta}{\partial P^4}, \frac{\partial^4 \mu}{\partial P^4} \in C\left([0, X_1] \times [0, P_{\max}]\right), \quad (3.9)$$

and if $t_s = sh, s = 0, \dots, N$ and $I_s = I(t_s)$, then

$$P(t_j) = P(t_{j-4}) + \frac{4}{3}h(2I_{j-3} - I_{j-2} + 2I_{j-1}) + E_1^j, \quad (3.10)$$

where $E_1^j \leq C_1 h^5$ and C_1 is constant, depending on $\max_{t \in [0, T]} \left| \frac{\partial^4 I(t)}{\partial t^4} \right|$, but independent of h, j .

If

$$\frac{\partial^4 u}{\partial x^4} \in C(\mathcal{S}), \frac{\partial^4 \beta}{\partial x^4}, \frac{\partial^4 \mu}{\partial x^4} \in C\left([0, X_1] \times [0, P_{\max}]\right) \quad (3.11)$$

then $I(t_s)$ are approximated as follows (recall that $x_K = X$),

$$I_s = -g(x_K)u(x_K, t_s) + \sum_{l=1}^K q_l[\beta(x_l, P(t_s)) - \mu(x_l, P(t_s))]u(x_l, t_s) + E_2^s, \quad s = 0, \dots, N \quad (3.12)$$

where $E_2^s \leq C_2 h^4$ and C_2 is a constant depending on

$$\max_{(x,t) \in \mathcal{S}} \left| \frac{\partial^i}{\partial x^i} \{ [\beta(x, P(t)) - \mu(x, P(t))] u(x, t) \} \right|, \quad i = 3, 4.$$

The coefficients q_l are calculated as:

$$\begin{aligned} q_r &= \int_0^{x_4} \frac{\omega_1(x)}{(x - x_r)\omega_1'(x_r)} dx, \quad r = 0, 1, 2, 3, 4, \\ q_{3s+r} &= \int_{x_{3s+4}}^{x_{3(s+1)+4}} \frac{\omega_{s+1}(x)}{(x - x_{3s+r})\omega_s'(x_{3s+r})} dx, \quad r \neq 4, \quad s = 0, \dots, M-1, \\ q_{3s+4} &= \int_{x_{3s}}^{x_{3s+4}} \frac{\omega_s(x)}{(x - x_{3s+4})\omega_s'(x_{3s+4})} dx + \int_{x_{3s+4}}^{x_{3(s+1)+4}} \frac{\omega_{s+1}(x)}{(x - x_{3s+4})\omega_{s+1}'(x_{3s+4})} dx, \quad s = 0, \dots, M-1, \end{aligned} \quad (3.13)$$

where

$$\omega_1(x) = (x - x_0) \dots (x - x_4), \quad \text{and} \quad \omega_s(x) = (x - x_{3s+4}) \dots (x - x_{3(s+1)+4}).$$

The sum in (3.12) represents the nonuniform rule.

Obviously, to apply the above formulae, we need to have approximations for $u(x_i, t_j)$. To this end, we need to assume also that

$$\frac{d^5 g}{dx^5} \in C([0, X_1]). \quad (3.14)$$

Then we can use a discretization of (2.2):

$$\begin{aligned} u(x_i, t_j) &= u(x_{i-2}, t_{j-2}) e^{-\frac{h}{3}[m(x_{i-2}, P(t_{j-2})) + 4m(x_{i-1}, P(t_{j-1})) + m(x_i, P(t_j))] + O(h^5)}, \quad L \geq i \geq 2, \quad N \geq j \geq 2 \\ u(x_1, t_j) &= u(0, t_{j-1}) e^{-\frac{h}{2}[m(x_0, P(t_{j-1})) + m(x_1, P(t_j))] + O(h^3)}, \\ u(0, t_j) &= \sum_{l=1}^K q_l \beta(x_l, P(t_j)) u(x_l, t_j) + O(h^4). \end{aligned} \quad (3.15)$$

The estimates of the discretization order rely on the assumption that the values at the preceding points (i.e. $P(t_{j-n}), u(x_{i-n}, t_{j-n})$) are known exactly. The expressions $O(h^q)$ above are used to denote the approximation errors, which are of the form $E_i^j \leq C_p h^q$ and C_p are constants independent of i, j and h but dependent on $\max_{(x,t) \in \mathcal{S}} \left| \frac{\partial^i}{\partial x^i} u(x, P(t)) \right|, i = 3, 4, \max_{(x,t) \in \mathcal{S}} \left| \frac{\partial^i}{\partial t^i} m(x, P(t)) \right|, i = 2, 4, \max_{(x,t) \in \mathcal{S}} \left| \frac{\partial^i}{\partial x^i} \{ \beta(x, P(t)) u(x, t) \} \right|, i = 2, 4.$

3.4 The Numerical Scheme

First we continue β and μ for negative values of P as

$$\beta(x, P) = \beta(x, -P), \quad \mu(x, P) = \mu(x, -P), \quad x \in [0, X_1], \quad P \in (-\infty, \infty).$$

Obviously, β and μ are bounded and nonnegative, $m = \mu + g'$ is nonnegative and $\frac{\partial \beta}{\partial P}$ and $\frac{\partial \mu}{\partial P}$ are continuous and bounded on $[0, X_1] \times (-\infty, \infty)$ with the exception of the line $P = 0$ where $\frac{\partial \beta}{\partial P}$ and $\frac{\partial \mu}{\partial P}$ may be discontinuous.

We introduce the grid functions $\tilde{u}_i^j, i = 0, \dots, L; j = 0, \dots, N$, defined on $\tilde{\mathcal{Z}}$ and \tilde{P}_j , defined on $I = \{0, \dots, t_N\}$. For $j \geq 4$ we use the following scheme to find the values of the grid functions, using the uniform and the nonuniform quadrature rules.

$$\tilde{P}_j = \tilde{P}_{j-4} + \frac{4}{3}h(2\tilde{I}_{j-3} - \tilde{I}_{j-2} + 2\tilde{I}_{j-1}), \quad (3.16)$$

where

$$\tilde{I}_s = -g(X)\tilde{u}_K^s + \sum_{l=1}^K \tilde{q}_l[\beta(y_l, \tilde{P}_s) - \mu(y_l, \tilde{P}_s)]\tilde{u}_l^s, \quad (3.17)$$

and \tilde{q}_l are defined by using formulae (3.13) with y_i instead of x_i .

$$\begin{aligned} \tilde{u}_i^j &= \tilde{u}_{i-2}^{j-2} e^{-\frac{h}{3}[m(y_{i-2}, \tilde{P}_{j-2}) + 4m(y_{i-1}, \tilde{P}_{j-1}) + m(y_i, \tilde{P}_j)]}, i \neq 0, 1, i \leq L, 4 \leq j \leq N; \\ \tilde{u}_1^j &= \tilde{u}_0^{j-1} e^{-\frac{h}{2}[m(y_1, \tilde{P}_j) + m(y_0, \tilde{P}_{j-1})]}, \\ \tilde{u}_0^j &= \sum_{l=1}^K \tilde{q}_l \beta(y_l, \tilde{P}_j) \tilde{u}_l^j. \end{aligned} \quad (3.18)$$

For $j = 0, 1, 2, 3$ we use initial values defined later through the *initialization process*.

3.5 An estimate for the global discretization error

In this section we show that the global discretization error of the numerical scheme depends on the accuracy of the initial values but is not better than $O(h^3)$. Let us denote:

$$\begin{aligned} \eta_j &= \tilde{P}_j - P(t_j); \\ \varepsilon_i^j &= \tilde{u}_i^j - u(x_i, t_j); \\ \zeta_j &= \tilde{I}_j - I_j; \\ \sigma_j &= h \sum_{l=1}^K |\varepsilon_l^j|, \\ i &= 0, \dots, L, j = 0, \dots, N. \end{aligned} \quad (3.19)$$

Theorem 3.1. *Consider the discretization scheme (3.16-3.18) with β and μ defined as in section 3.4. Suppose that the assumptions (3.9), (3.11) and (3.14) hold. Then for $j \geq 4$ the following discretization error estimates hold:*

$$|\eta_j| \leq W_1 h^3 + W_2 \left(\max_{i=0,1,2,3} |\eta_i| + \max_{l=0,\dots,L} \max_{j=0,1,2,3} |\varepsilon_l^j| \right), \quad (3.20)$$

$$|\varepsilon_i^j| \leq W_3 h^3 + W_4 \left(\max_{i=0,1,2,3} |\eta_i| + \max_{l=0,\dots,L} \max_{j=0,1,2,3} |\varepsilon_l^j| \right), \quad (3.21)$$

where $W_s, s = 1, 2, 3, 4$ are constants, independent of h, j, i .

Proof: Subtracting (3.10) from (3.16), we get

$$|\eta_j| \leq |\eta_{j-4}| + \frac{4}{3} h [2\zeta_{j-3} - \zeta_{j-2} + 2\zeta_{j-1}] + C_1 h^5, \quad j \leq N. \quad (3.22)$$

Subtracting (3.12) from (3.17), we get:

$$\begin{aligned} |\zeta_s| \leq g(X) |\varepsilon_K^s| + \sum_{l=1}^K |(q_l - \tilde{q}_l) |\beta_l^s u_l^s + \tilde{q}_l \tilde{\beta}_l |\varepsilon_l^s| + \tilde{q}_l u_l^s |\beta_l^s - \tilde{\beta}_l^s| + \\ \sum_{l=1}^K |(q_l - \tilde{q}_l) |\mu_l^s u_l^s + \tilde{q}_l \tilde{\mu}_l |\varepsilon_l^s| + \tilde{q}_l u_l^s |\mu_l^s - \tilde{\mu}_l^s| + C_2 h^4, \end{aligned} \quad (3.23)$$

where we have denoted $f_l^s = f(x_l, P(t_s)), \tilde{f}_l^s = f(x_l, \tilde{P}_s)$.

Taking into consideration that $\beta, \mu, \frac{\partial \beta}{\partial P}, \frac{\partial \mu}{\partial P}$ and $u(x, t)$ are bounded, and that

$$\tilde{q}_l = O(h), \quad |(q_l - \tilde{q}_l)| = O(h^5) \text{ and } |x_l - y_l| = O(h^4), \quad (3.24)$$

we can write

$$|\zeta_s| \leq g(X) |\varepsilon_K^s| + A |\eta_s| + B |\sigma_s| + C_2 h^4, \quad (3.25)$$

where A, B, C_1, C_2 are positive constants, independent of h and s . In the derivation of the above estimate we have used also that $\frac{\partial \beta}{\partial P}, \frac{\partial \mu}{\partial P}$ are continuous with the exception of the line $P = 0$. It is easy to see that the possible discontinuity is not an obstacle to the derivation of the estimate.

In what follows we assume without loss of generality that the step h is less than some maximum value, say h_{\max} . Each time when we use the expression "the constant C is independent of h ", the meaning is "the constant C is the same for all $h \leq h_{\max}$ ". If $C_3 = C_1 h_{\max} + C_2$, then

$$\begin{aligned} |\eta_j| \leq |\eta_{j-4}| + \frac{4}{3} h \{ A [2|\eta_{j-3}| + |\eta_{j-2}| + 2|\eta_{j-1}|] + \\ B [2|\sigma_{j-3}| + |\sigma_{j-2}| + 2|\sigma_{j-1}|] + \\ g(X) [2|\varepsilon_K^{j-3}| + |\varepsilon_K^{j-2}| + 2|\varepsilon_K^{j-1}|] \} + C_3 h^4, \end{aligned} \quad (3.26)$$

and C_3 is independent of h and j .

Subtracting (3.15) from (3.18) and taking into consideration that $m \geq 0$ and $\frac{\partial \beta}{\partial P}$ and $\frac{\partial \mu}{\partial P}$ are bounded and (3.24) we get

$$\begin{aligned} |\varepsilon_i^j| &\leq |\varepsilon_{i-2}^{j-2}| + hD [|\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_4 h^5, \quad i, j > 1; \\ |\varepsilon_1^j| &\leq |\varepsilon_0^{j-1}| + hH [|\eta_{j-1}| + |\eta_j|] + C_6 h^3; \\ |\varepsilon_0^j| &\leq G |\eta_j| + P |\sigma_j| + C_7 h^4, \end{aligned} \quad (3.27)$$

where $C_i, i = 0, 4, \dots, 7, D, H, G, P$ are positive constants independent of h and j .

By substituting the estimate for $|\varepsilon_0^j|$ in the first 2 inequalities of (3.27), we get

$$\begin{aligned} |\varepsilon_1^j| &\leq G|\eta_{j-1}| + P|\sigma_{j-1}| + hH[|\eta_{j-1}| + |\eta_j|] + C_8h^3; \\ |\varepsilon_2^j| &\leq G|\eta_{j-2}| + P|\sigma_{j-2}| + hD[|\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_9h^4; \\ |\varepsilon_3^j| &\leq G|\eta_{j-3}| + P|\sigma_{j-3}| + hF[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{10}h^4, \end{aligned} \quad (3.28)$$

where F and $C_i, i = 8, \dots, 10$ are positive constants independent of h, j .

From (3.27₁) we get that for $i \geq 4, j \geq 4$ it holds:

$$|\varepsilon_i^j| \leq |\varepsilon_{i-4}^{j-4}| + 2hD[|\eta_{j-4}| + |\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{11}h^5. \quad (3.29)$$

We now consider $|\varepsilon_K^s|$ and reiterate (3.27₁) until we get for $s \geq K$

$$|\varepsilon_K^s| \leq \dots \leq |\varepsilon_{s-K+\alpha}^{s-K+\alpha}| + 2hD\{|\eta_{s-K+\alpha}| + \dots + |\eta_s|\} + C_{11}^1h^4, \quad (3.30)$$

and for $s < K$:

$$|\varepsilon_K^s| \leq \dots \leq |\varepsilon_{K-s+\alpha}^{\alpha}| + 2hD\{|\eta_{\alpha}| + \dots + |\eta_s|\} + C_{11}^1h^4, \quad (3.31)$$

where α takes the value 0 or 1 and $C_{11}^1 = C_{11}Nh = C_{11}T$.

If $s \geq K$, (3.28) and (3.27) give:

$$|\varepsilon_{\alpha}^{s-K+\alpha}| \leq G|\eta_{s-K}| + P|\sigma_{s-K}| + hH(|\eta_{s-K}| + |\eta_{s-K+1}|) + C_{11}^2h^3, \quad \alpha = 0, 1. \quad (3.32)$$

If $s < K$, $|\varepsilon_{K-s+\alpha}^{\alpha}|$ is of the order determined by the initialization process (see next section).

We combine (3.30) and (3.31) using (3.32) to write:

$$|\varepsilon_K^s| \leq G|\eta_{s-K}| + P|\sigma_{s-K}| + 2hD_1(|\eta_s| + \dots + |\eta_0|) + |\varepsilon_{K-s}^0| + |\varepsilon_{K-s+1}^1| + C_{11}^3h^3, \quad (3.33)$$

where $\varepsilon_{\gamma}^{\delta} = 0, \eta_{\kappa} = 0, \sigma_{\kappa} = 0$ whenever $\gamma < 0$, or $\kappa < 0$.

Therefore from (3.26) and (3.33) we get:

$$\begin{aligned} |\eta_j| &\leq |\eta_{j-4}| + \frac{8}{3}h \left\{ A[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}|] + B[|\sigma_{j-3}| + |\sigma_{j-2}| + |\sigma_{j-1}|] + \right. \\ &\quad \left. g(X) \left[G(|\eta_{j-3-K}| + |\eta_{j-2-K}| + |\eta_{j-1-K}|) + P(|\sigma_{j-3-K}| + |\sigma_{j-2-K}| + |\sigma_{j-1-K}|) \right] \right\} + \\ &\quad g(X) \left\{ 8h \left(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1| \right) + 16Dh^2[|\eta_{j-1}| + \dots + |\eta_0|] \right\} + C_{11}^4h^4, \end{aligned} \quad (3.34)$$

where $\eta_{\kappa} = 0, \sigma_{\kappa} = 0$ whenever $\kappa < 0$.

Let $j \geq 4$. Summing up (3.28) and (3.29) for $i \geq 4$, multiplying the sum by h , and renaming some constants, we get

$$\begin{aligned} |\sigma_j| &\leq |\sigma_{j-4}| + hP[|\sigma_{j-1}| + |\sigma_{j-2}| + |\sigma_{j-3}|] + hG[|\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}|] \\ &\quad + h^2Q[|\eta_{j-4}| + |\eta_{j-3}| + |\eta_{j-2}| + |\eta_{j-1}| + |\eta_j|] + C_{12}h^4. \end{aligned} \quad (3.35)$$

In the last several expressions, $Q, D_1, C_{11}, C_{11}^1, C_{11}^2, C_{11}^3, C_{11}^4$ and C_{12} are positive constants independent of h, j .

Let us denote $\rho_j = |\sigma_j| + |\eta_j|$.

We rewrite (3.34) as

$$|\eta_j| \leq |\eta_{j-4}| + hU_1(\rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + hU_2(\rho_{j-3-K} + \rho_{j-2-K} + \rho_{j-1-K}) + h^2U_3(|\eta_{j-1}| + \dots + |\eta_0|) + Rh(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|) + C_{11}^4 h^4. \quad (3.36)$$

where U_i and R are constants, independent of j, h .

We substitute $|\eta_j|$ in (3.35) with its upper estimate, and write:

$$|\sigma_j| \leq |\sigma_{j-4}| + hV_1(\rho_{j-4} + \rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + h^2Q\{|\eta_{j-4}| + hU_1(\rho_{j-3} + \rho_{j-2} + \rho_{j-1}) + hU_2(\rho_{j-3-K} + \rho_{j-2-K} + \rho_{j-1-K}) + h^2U_3(|\eta_{j-1}| + \dots + |\eta_0|) + C_{11}^3 h^4\} + RQh^3(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|) + C_{12}^1 h^4. \quad (3.37)$$

where C_{12}^1, V_i are constants, independent of j, h .

We now add (3.36) and (3.37) to obtain after renaming some constants:

$$\rho_j \leq \rho_{j-4} + hY_1[\rho_{j-1} + \rho_{j-2} + \rho_{j-3} + \rho_{j-4} + \rho_{j-1-K} + \rho_{j-2-K} + \rho_{j-3-K}] + h^2Y_2(\rho_{j-1} + \dots + \rho_0) + hS(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|) + C_{13}h^4, \quad (3.38)$$

where S is a constant independent of h and j and $\rho_\alpha = 0$, whenever $\alpha < 0$.

Reiterating the inequality and renaming some constants we get

$$\rho_j \leq \rho_{q_j} + ST(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|) + hZ[\rho_{j-1} + \dots + \rho_0] + C_{14}h^3, \quad (3.39)$$

where Z, C_{13}, C_{14} and Y_1, Y_2 are positive constants independent of h, j and q_j is an integer taking one of the values 0, 1, 2 or 3.

Applying a discrete Gronwall inequality, [6], p.41, we conclude that

$$\begin{aligned} \rho_j &\leq \left\{ C_{14}h^3 + \rho_{q_j} + ST(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|) \right\} (1 + hZ)^j < \\ &[C_{14}h^3 + \rho_{q_j} + ST(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|)] (1 + \frac{T}{N}Z)^N < \\ &[C_{14}h^3 + \rho_{q_j} + ST(\max_{0 \leq n \leq K} |\varepsilon_n^0| + \max_{0 \leq n \leq K} |\varepsilon_n^1|)] e^{TZ}. \end{aligned} \quad (3.40)$$

Since

$$\max_{j=0,1,2,3} \rho_{q_j} \leq \max_{j=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0, \dots, K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)|,$$

then

$$\begin{aligned} |\eta_j| &\leq \left\{ C_{14}h^3 + \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + (1 + ST) \max_{l=0, \dots, K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)| \right\} e^{TZ}, \\ |\sigma_j| &\leq \left\{ C_{14}h^3 + \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + (1 + ST) \max_{l=0, \dots, K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)| \right\} e^{TZ}. \end{aligned} \quad (3.41)$$

Let us turn back now to (3.27), denoting $1 + ST = S_*$.

$$\begin{aligned} |\varepsilon_i^j| &\leq |\varepsilon_{i-2}^{j-2}| + 3hD \left\{ C_{14}h^3 + S_* \max_{i=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0,\dots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)| \right\} e^{TZ} + C_4h^5 \\ &\leq |\varepsilon_{r_i}^{p_j}| + C_{15}h^3 + C_{16} \left\{ \max_{j=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0,\dots,K} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)| \right\}, \end{aligned} \quad (3.42)$$

where C_{15} and C_{16} are positive constants independent of h, j and r_i and p_j take the values 0 or 1.

Taking into consideration the last equation in (3.27) and the first one of (3.28) together with (3.41), we conclude that

$$|\varepsilon_i^j| \leq C_{17}h^3 + C_{18} \left\{ \max_{j=0,1,2,3} |\tilde{P}_i - P(t_i)| + \max_{l=0,\dots,L} \max_{j=0,1,2,3} |\tilde{u}_l^j - u(x_l, t_j)| \right\}, \quad (3.43)$$

where C_{17} and C_{18} are positive constants independent of h, j .

This concludes the proof. \square

So, the global error of the method depends on the local error of the first 4 time layers, but cannot be of order higher than 3. Mind that the 3rd order of the discretization error occurred only because ε_i^j is of that order.

In the next section we show how we can find initial approximations for the first several time layers.

3.6 The initialization

We shall first find approximations with sufficient accuracy for P and u at $t = 0, h, 2h, 3h$. We first calculate

$$\tilde{P}_0 = \sum_{l=1}^K \tilde{q}_l u_0(y_l). \quad (3.44)$$

Obviously,

$$\tilde{P}_0 = P(0) + O(h^4).$$

The error comes from the numerical quadrature and the inaccuracy of the nodes and the coefficients q_l .

Further, we calculate

$$\tilde{P}_1 = \tilde{P}_0 - hg(X)u_0(X) + h \sum_{l=1}^K \tilde{q}_l [\beta(y_l, \tilde{P}_0) - \mu(y_l, \tilde{P}_0)]u_0(y_l) \quad (3.45)$$

Then $\tilde{P}_1 - P(t_1) = O(h^2)$.

Further,

$$\tilde{u}_i^1 = u_0(y_{i-1})e^{-\frac{h}{2}[m(y_{i-1}, \tilde{P}_0) + m(y_i, \tilde{P}_1)]}, \quad i = 1, \dots, L,$$

for which one can establish easily that

$$|\tilde{u}_i^1 - u(x_i, t_1)| = O(h^3).$$

Let $\tilde{P}_1 = P_1^{old}$ and let us apply a trapezoid rule in time and an open nonuniform rule in space.

$$\begin{aligned} \tilde{P}_1 = & \tilde{P}_0 + \frac{h}{2} \left\{ -g(X)[u_0(X) + \tilde{u}_K^1] + \sum_{l=1}^K \tilde{q}_l[\beta(y_l, \tilde{P}_0) - \mu(y_l, \tilde{P}_0)]u_0(y_l) \right. \\ & \left. + \sum_{l=1}^K \tilde{q}_l[\beta(y_l, \tilde{P}_1^{old}) - \mu(y_l, \tilde{P}_1^{old})]\tilde{u}_l^1 \right\}. \end{aligned} \quad (3.46)$$

One can establish that the new value of \tilde{P}_1 is more accurate:

$$\tilde{P}_1 - P(t_1) = O(h^3).$$

We cannot improve the accuracy of u_i^1 anymore, however, because the third order error comes from the trapezoid rule in the exponential. A more accurate rule cannot be applied at this layer (first t -layer) because we do not have more than 2 available values of P .

Note that we applied a procedure of step by step accuracy refinement by first finding approximate values for P , using them to calculate approximations for u and then refining the approximation for P again. Theoretically, one can use the new values to refine the approximations for u , but as we already saw, this "PuP"- procedure gives result only a finite number of times.

We calculate finally

$$\tilde{u}_0^1 = \sum_{l=1}^K \tilde{q}_l \beta(y_l, \tilde{P}_1) \tilde{u}_l^1 = u(0, h) + O(h^3). \quad (3.47)$$

Now we find \tilde{P}_2 by using the midpoint rule in the discretization of the time integrals:

$$\tilde{P}_2 = \tilde{P}_0 - 2h \left\{ g(X) \tilde{u}_K^1 + \sum_{l=1}^K \tilde{q}_l[\beta(y_l, \tilde{P}_1) - \mu(y_l, \tilde{P}_1)]\tilde{u}_l^1 \right\}, \quad (3.48)$$

which can be written as

$$\tilde{P}_2 = \tilde{P}_0 + 2h\tilde{I}_1.$$

Then one can find that

$$|\tilde{P}_2 - P(t_2)| = O(h^3).$$

Further, u_i^2 is calculated as

$$\begin{aligned} \tilde{u}_i^2 &= u_0(y_{i-2})e^{-\frac{h}{3}[m(y_{i-2}, \tilde{P}_0) + 4m(y_{i-1}, \tilde{P}_1) + m(y_i, \tilde{P}_2)]}, \text{ for } i \geq 2, \\ \tilde{u}_1^2 &= u_0(0)e^{-\frac{h}{2}[m(0, \tilde{P}_0) + m(y_1, \tilde{P}_1)]}. \end{aligned} \quad (3.49)$$

One can find that

$$\begin{aligned} \tilde{u}_i^2 &= u(x_i, t_2) + O(h^4), \quad i \geq 2, \\ \tilde{u}_1^2 &= u(x_1, t_2) + O(h^3). \end{aligned} \quad (3.50)$$

We do the "PuP-procedure" to calculate \tilde{P}_2 using these values of u_l^2 using Simpson's rule.

$$\tilde{P}_2 = \tilde{P}_0 + \frac{h}{6}[\tilde{I}_0 + 4\tilde{I}_1 + \tilde{I}_2^{old}], \quad (3.51)$$

where \tilde{I}_2^{old} is calculated according to formula (3.17) but with the value P_2^{old} instead of \tilde{P}_2 .

One can see that

$$\tilde{P}_2 = P(t_2) + O(h^4).$$

Further, we recalculate $\tilde{u}_i^2, i = 1, \dots, L$ using formula (3.49) with the so found P_2 . We obtain new values $\tilde{u}_i^2, i = 2, \dots, L$:

$$\tilde{u}_i^2 = u(x_i, t_2) + O(h^4),$$

and

$$\tilde{u}_1^2 = u(x_1, t_2) + O(h^3).$$

Finally, we calculate u_0^2 :

$$\tilde{u}_0^2 = \sum_{l=1}^K \tilde{q}_l \beta(y_l, \tilde{P}_2) \tilde{u}_l^2, \quad (3.52)$$

thus obtaining that

$$\tilde{u}_0^2 = u(0, t_2) + O(h^4).$$

We continue to obtain \tilde{P}_3 by using a 4 - point open formula R_{open} to approximate the time integrals:

$$\tilde{P}_3 = \tilde{P}_0 + \frac{3h}{2}[\tilde{I}_1 + \tilde{I}_2], \quad (3.53)$$

thus obtaining

$$\tilde{P}_3 = P(t_3) + O(h^3).$$

We further calculate $\tilde{u}_i^3, i = 3, \dots, L$ as

$$\tilde{u}_i^3 = u_{i-3}^0 e^{-\frac{3h}{8}[m(y_{i-3}, \tilde{P}_0) + 3m(y_{i-2}, \tilde{P}_1) + 3m(y_{i-1}, \tilde{P}_2) + m(y_i, \tilde{P}_3)]},$$

thus obtaining local approximation of order $O(h^4)$.

$$\tilde{u}_i^3 = u(x_i, t_3) + O(h^4), i = 3, \dots, L.$$

The values \tilde{u}_1^3 and \tilde{u}_2^3 can be only calculated with $O(h^3)$ accuracy:

$$\begin{aligned} \tilde{u}_1^3 &= u_0^2 e^{-\frac{h}{2}[m(0, \tilde{P}_2) + m(y_1, \tilde{P}_3)]} = u(x_1, P(t_3)) + O(h^3) \\ \tilde{u}_2^3 &= u_1^2 e^{-\frac{h}{2}[m(y_1, \tilde{P}_2) + m(y_2, \tilde{P}_3)]} = u(x_2, P(t_3)) + O(h^3) \end{aligned} \quad (3.54)$$

The "PuP-procedure" will give a better estimate for P_3 now by using a 4-point closed rule $F_{\frac{3}{8}}$ for the time integral:

$$\tilde{P}_3 = \tilde{P}_0 + \frac{3h}{8}[\tilde{I}_0 + 3\tilde{I}_1 + 3\tilde{I}_2 + \tilde{I}_3^{old}] = P(t_3) + O(h^4), \quad (3.55)$$

where \tilde{I}_3^{old} has an obvious meaning.

No further improvement in the accuracy of \tilde{u}_i^3 can be achieved, so we proceed to calculating \tilde{u}_0^3 ,

$$\tilde{u}_0^3 = \sum_{l=1}^K \tilde{q}_l \beta(y_l, \tilde{P}_3) \tilde{u}_l^3 = u(0, t_3) + O(h^4). \quad (3.56)$$

This concludes the initialization process.

3.7 The magnitude of the global discretization error

Combining the results of the initialization process and Theorem 3.1, we can formulate the following result.

Theorem 3.2. *If the assumptions of Theorem 3.1 hold, the global discretization error of the numerical scheme (3.16-3.18) combined with the initialization described in section 3.6 is of the order $O(h^3)$.*

Going through the proof of Theorem 3.1 we can notice that the 3rd order of the global error is actually due to the 3rd order discretization error in the calculation of $u(h, t_j)$. If this layer could be calculated with a better accuracy, the algorithm would benefit by producing a higher order of the global error.

4 Implementation of the Numerical Algorithm

A Fortran code implementing the proposed algorithm was written by the author and is available upon request. It works for problems with $X = X_1 = 1$, but can be easily modified for a larger class of problems.

The method was tested on the following example.

$$\begin{aligned} u_t + (e^{-x}u)_x &= -(1 + e^{-x} + \frac{e^{-x} \sin x}{2 + \cos x})u, \quad x \in (0, 1], t > 0, \\ u(0, t) &= \int_0^1 \frac{3}{2 + \cos x} u(x, t) dx \\ u(x, 0) &= 1 + \frac{\cos x}{2}, \end{aligned} \quad (4.1)$$

which has the exact solution $u(x, t) = e^{-t}(1 + \frac{\cos x}{2})$.

The solution was calculated for $t \in [0, 69]$ with 4 different values of the step. The code calculates the grid by solving (2.1) by a Runge-Kutta 4th order method. The following table reports a summary of the numerical results in terms of the maximum error $\eta_{\max} = \max_{j=0, \dots, N} |\eta_j|$, $\varepsilon_{\max} = \max_{i,j} |\varepsilon_i^j|$ and the average error $\eta_{av} = \frac{1}{N+1} \sum_{k=0}^N |\eta_k|$, $\varepsilon_{av} = \frac{\sum_{i=1, \dots, L, j=1, \dots, N} |\varepsilon_i^j|}{N \cdot L}$. The experimental results agree closely with the theoretical ones.

Table 1. Amount of the error for various h

Step h	η_{\max}	η_{av}	ε_{\max}	ε_{av}
0.09044	6.83×10^{-4}	1.24×10^{-4}	1.25×10^{-4}	9.8×10^{-7}
0.0505	1.27×10^{-4}	1.93×10^{-5}	2.75×10^{-5}	1.59×10^{-7}
0.0268	1.97×10^{-5}	2.54×10^{-6}	4.67×10^{-6}	2.1×10^{-8}
0.0139	3.13×10^{-6}	4.68×10^{-7}	1.096×10^{-6}	8.75×10^{-9}

5 Discussion

Note that, to apply the method, we needed to continue μ and β for negative P and to assume boundedness of $\beta, \mu, \frac{\partial \beta}{\partial P}, \frac{\partial \mu}{\partial P}$ for all P . The problem (1.1) by itself requires that the vital rates are defined only for $P \geq 0$. The continuation of β, μ becomes necessary in case that the solution tends to 0 and negative values of \tilde{P}_i might appear, although these would be good approximations of $P(t_i)$.

A similar method which will always generate positive P_i (and therefore a continuation of β, μ will not be needed) can be proposed. It can be one that utilizes a different formula for the time discretization (3.10) of P . Such a formula can be

$$P(t_j) = P(t_{j-5}) + h \frac{5}{24} (11I_{j-4} + I_{j-3} + I_{j-2} + 11I_{j-1}),$$

based on the quadrature rule

$$\int_{x_0}^{x_5} f(x) dx = h \frac{5}{24} [11f(x_1) + f(x_2) + f(x_3) + 11f(x_4)] - \frac{95}{144} f^{(4)}(\zeta) h^5.$$

The error analysis will go along the same line as in Theorem 3.1. The price to be paid for using such a formula is to calculate one more initial time layer with accuracy $O(h^4)$. Such a method will not ease the requirements for boundedness of β, μ and their P - derivatives.

References

- [1] L.M. Abia and J.C. Lopez-Marcos, (1995) Runge-Kutta methods for age-structured population models, *Applied Num. Math.*, **17**: 1-17
- [2] Angulo, O. and J.C. Lopez-Marcos, (1998) Numerical Schemes for Size-Structured Population Models, *Mathematical Biosciences*, **157**: 169-188
- [3] Angulo, O. and J.C. Lopez-Marcos, (1998) Numerical Integration of Nonlinear Size-Structured Population Equations, *Report of the Department of Applied Mathematics, Polytechnical University, Universidad de Valladolid*
- [4] T. Arbogast and F.A. Milner, (1989) A finite element method for a two-sex model of population dynamics, *SIAM J. Numer. Anal.* **26**: 1474-1486
- [5] T. H. Barr, (1991) Approximation for Age-Structured Population Models Using Projection Methods, *Computers, Math. , Applic.*, **21**, no. 5: 17-40

- [6] H. Brunner, P.J. van der Houwen, (1986) *The Numerical Solution of Volterra Equations*, *CWI Monograph 3*, North Holland, Amsterdam
- [7] J. Douglas, Jr., and F.A. Milner, (1987) Numerical methods for a model of population dynamics, *Calcolo* **24**: 247-254
- [8] G. Fairweather, (1991) A box method for a non linear equation of population dynamics, *IMA Journal of Numerical Analysis* **11**: 525-538
- [9] G. Fairweather and J.C. Lopez-Marcos, (1994) An explicit extrapolated box scheme for the Gurtin-MacCamy equation, *Computers Math. Applic.* **27**: 41-53
- [10] Iannelli, M., *Mathematical Theory of Age - Structured Population Dynamics*, Appl. Mathematical Monographs, C.N.R.I (1995)
- [11] Ito, K., F. Kappel and G. Peichl, (1991) A Fully Discretized Approximation Scheme for Size-Structured Population Models, *SIAM J. Numer. Anal.* **28**: 923-954
- [12] F. Kappel and K. Zhang, (1993) Approximation of Linear Age-Structured Population Models Using Legendre Polynomials, *J. Math. Anal. and Appls.*, **180**: 518-549
- [13] T.V. Kostova, (1988) Numerical solutions of a hyperbolic differential-integral equation, *Computers Math. Applic.* **15**: 427-436
- [14] T.V. Kostova, (1990) Numerical solutions to equations modelling nonlinearly interacting age-dependent populations, *Computers Math. Applic.* **18**: 95-103
- [15] J.C. Lopez-Marcos, (1991) An upwind scheme for a nonlinear hyperbolic integro-differential equation with integral boundary condition, *Computers Math. Applic.* **22**: 15-28
- [16] F.A. Milner and G. Rabbio, (1992) Rapidly converging numerical algorithms for models of population dynamics, *J. Math. Biol.* **30**: 733-753
- [17] Webb, G. F., *Theory of Age Dependent Population Dynamics*, Marcel Dekker, New York, (1985).