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FOURTH-ORDER METHOD FOR NUMERICAL INTEGRATION OF AGE- AND SIZE-STRUCTURED POPULATION MODELS

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Abstract

In many applications of age- and size-structured population models, there is an interest in obtaining good approximations of total population numbers rather than of their densities. Therefore, it is reasonable in such cases to solve numerically not the PDE model equations themselves, but rather their integral equivalents. For this purpose quadrature formulae are used in place of the integrals. Since quadratures can be designed with any order of accuracy, one can obtain numerical approximations of the solutions with very fast convergence. In this paper we present a general framework and a specific example of a fourth-order method based on composite Newton-Cotes quadratures for a size-structured population model.

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1 Introduction

Age- and size-structured models have evolved from the simple, unstructured ones that date back to Malthus's model of the late XVIIIth century that consisted of just a single ordinary differential equation. Modern models may involve several interacting populations (predator-prey models, species competing for resources, etc.) and/or internal structures of a single population through discrete (e.g. epidemic class, gender, race) or continuous variables (e.g. age, size, duration of infection).

When solved numerically, such systems can require considerable time and memory as they usually consist of combinations of ordinary and partial differential equations and integral equations that depend on several independent variables.

The published numerical methods for the approximation of the solutions to these models fall into one of three categories: methods based on the explicit analytic form of the solution by integration along characteristics, finite difference methods of characteristics, and finite difference methods for first order hyperbolic equations. All of these address the problem of approximating the age or size density of the population directly (solution of a partial differential equation) rather than the total population size and total birth rate, for example. For a very thorough review of published numerical methods for these models we refer the reader to [2].

An excellent source for a summary description of published methods for size-structured equations and some of their main features is [1].

Just to mention a few of the methods published, when the model is linear, i.e. linear μ, β, [12] uses spline functions and trapezoidal rule; [4] describes a numerical scheme based on Runge-Kutta methods along the characteristics. For nonlinear equations [5] provides a

continuation of the previous paper [4] that generalizes the method described therein using Runge-Kutta methods on the characteristics coupled with iterations to resolve the nonlinearities.

The third-order explicit method for nonlinear size-structured equations, presented in [13] is based on a combination of a discretization along the characteristics of the equation for u and a discretization of a differential equation for P.

However, when performing numerical simulations, we are often not so interested in the values of the density functions as in the values of the total population number or the size of certain age- or size-classes. Therefore, in such instances it is reasonable to solve numerically not the partial differential equations themselves, but rather their integral equivalent formulation. For this purpose, numerical methods that use quadrature formulae in place of the integrals can be designed. Since quadratures can be computed with any order of accuracy when the integrand is a smooth function, in such cases we can obtain numerical approximations of the solutions to the integral model equations with fast convergence. Moreover, integral equation methods frequently require less regularity of the solution than partial differential equation methods do. The main purpose of the present work is to describe numerical methods based on integral equations that model age- and size-structured population dynamics.

2 The Model Partial Differential Equations and Their Integral Equivalent

The classical size-structured model we shall consider has the following form:

$$\begin{cases} u_t + g(x)u_x = -\mu(x, P(t))u(x,t) \\ u(0,t) = B(t) = \displaystyle\int_0^A \beta(x, P(t))u(x,t)dx \\ u(x,0) = \phi(x), \end{cases} \tag{2.1}$$

where $t \in [0,T],\ x \in [0,A]$. The dependent variable $u(x,t)$ is the size-density of the population at time t, while $P(t) = \int_0^A u(x,t)dx$ represents the size of the whole population; $g(x)$ is called the growth function and is assumed that $g(x) > 0, x \in [0,1)$. Some authors assume that $g(x) \to 0$ as $x \to A$ to ensure that individuals do not grow infinitely. We shall not impose this requirement but, in the case when it is satisfied, we shall assume that the initial distribution has compact support $[0,a^*] \subset [0,A)$—that is, if $g(A) = 0$, then $\phi(x) = 0$ for $a^* \leq x < A$.

For simplicity and with no loss of generality, we assume that $A = 1$.

For the purpose of our analysis, we shall assume that all coefficients in (2.1), β, μ, and g possess sufficiently many derivatives in all their variables.

We remark that in the case $g(x) \equiv 1$, the resulting model is the usual age-structured one due to McKendrick and von Foerster [14],[16] in its nonlinear form studied by Gurtin and MacCamy [10].

The growth function $g(x)$ describes the rate of change of size in time, so that the characteristic curves in the xt-plane starting at points on the boundary of the first quadrant, Γ,

satisfy the equation

$$\frac{dx}{dt} = g(x), \tag{2.2}$$

with initial condition

$$\begin{aligned} &(x_0, t_0) \in \Gamma = \Gamma_1 \cup \Gamma_2, \\ &\Gamma_1 = \{x = 0, t \geq 0\}, \quad \Gamma_2 = \{x \geq 0, t = 0\}. \end{aligned} \tag{2.3}$$

Obviously, the solution of (2.2) is

$$t - t_0 = \int_{x_0}^{x} \frac{1}{g(x)} dx. \tag{2.4}$$

Let $\theta(x; x_0, t_0) = t = t_0 + \int_{x_0}^{x} \frac{1}{g(s)} ds$, and note that this is an increasing function. Let $\chi(t; x_0, t_0) = \theta^{-1}(t; x_0, t_0)$ denote the inverse function of θ. We now have that both representations

$$\mathcal{C}(x_0, t_0) = \Big\{ t = \theta(x; x_0, t_0),\ x \in [0, 1) \Big\} = \Big\{ x = \chi(t; x_0, t_0),\ t \in [0, T) \Big\}$$

describe the characteristic curve starting at $(x_0, t_0) \in \Gamma$. The characteristic $\mathcal{C}(0, 0)$ has a special significance. It separates the set of charateristic curves starting on Γ_1 from those starting on Γ_2. To simplify our notation, denote $\sigma(t) = \chi(t; 0, 0)$, i.e. $\mathcal{C}(0, 0) = \Big\{ x = \sigma(t),\ t \in [0, T) \Big\}$.

Denote by $\mathcal{S}$ the rectangle in which the solution of (2.1) is sought,

$$\mathcal{S} = \big\{ (x, t) : x \in [0, A),\ t \in [0, T] \big\}.$$

Proposition 2.1. *To each pair $(x, t) \in \mathcal{S}$, there corresponds a unique pair $(x_0, t_0) \in \Gamma$, such that $(x, t) \in \mathcal{C}(x_0, t_0)$ and such that if $x \leq \sigma(t)$, then $(x_0, t_0) \in \Gamma_1$ and if $x > \sigma(t)$, then $(x_0, t_0) \in \Gamma_2$.*

Proof. It is obvious that if such a pair $(x_0, t_0) \in \Gamma$ exists, it is unique.

a) If $t-\int_0^x \frac{1}{g(s)}ds \geq 0$, i.e. if $x \leq \sigma(t)$, then $x_0(x,t)=0,\ t_0(x,t)=t-\int_0^x \frac{1}{g(s)}ds=\theta(0;x,t)$, satisfies (2.4). Obviously, $(x_0,t_0)\in\Gamma_1$.

b) If $t-\int_0^x \frac{1}{g(s)}ds < 0$, i.e. if $x > \sigma(t)$, then we check that $x_0(x,t)=\chi(0;x,t),\ t_0(x,t)=0$ satisfy (2.4) i.e. $(x_0,t_0)\in\Gamma_2$.

∎

Proposition 2.2. *The solution of (2.1) can be written as*

$$u(x,t)=\begin{cases} B\big(\theta(0;x,t)\big)\, e^{-\int_{\theta(0;x,t)}^{t}\mu(\chi(\tau;0,\theta(0;x,t)),P(\tau))\,d\tau}, & \text{if } x<\chi(t;0,0),\\ \phi\big(\chi(0;x,t)\big)\, e^{-\int_0^t \mu(\chi(\tau;\chi(0;x,t),0),P(\tau))d\tau}, & \text{if } x>\chi(t;0,0). \end{cases} \tag{2.5}$$

Proof. The technique of integration along characteristics is used.

Let $(x,t)\in\mathcal{S}$. We take $x_0=x_0(x,t),\ t_0=t_0(x,t)$ as the unique pair $(x_0,t_0)\in\Gamma$ that lies on the characteristic curve through (x,t). Then $u(x,t)=u(\chi(t;x_0,t_0),t)$. Let $\omega(t)=u(\chi(t;x_0,t_0),t)$. Then $\omega(t)$ obeys the first-order equation

$$\omega'(t)=u_x(\chi(t;x_0,t_0),t)\,g(\chi(t;x_0,t_0))+u_t(\chi(t;x_0,t_0),t)=-\mu\big(\chi(t;x_0,t_0),P(t)\big)\,\omega(t), \tag{2.6}$$

which can be solved "implicitly" due to the presence of $P(t)$ in the right-hand side of (2.6). According to Proposition 2.1,

$$\omega(t_0)=u(x_0,t_0)=\begin{cases} B(t_0)=B(\theta(0;x,t)), & \text{if } (x_0,t_0)\in\Gamma_1,\\ \phi(x_0)=\phi(\chi(0;x,t)), & \text{if } (x_0,t_0)\in\Gamma_2. \end{cases} \tag{2.7}$$

Integrating the ODE (2.6) and using the initial condition (2.7), we obtain (2.5).

∎

Equation (2.5) is a generalization of a similar integral form in the case of age-structured systems [11], when $g\equiv 1$ that has not been derived in detail previously.

Note that equation (2.5) can be written in the concise form

$$u(x,t) = \begin{cases} \mathcal{U}_B(\theta(0;x,t),t), & \text{if } x < \chi(t;0,0), \\ \mathcal{U}_\phi(\chi(0;x,t),t), & \text{if } x > \chi(t;0,0), \end{cases} \tag{2.8}$$

where

$$\begin{aligned} \mathcal{U}_B(z,t) &= B(z)e^{-\int_z^t \mu(\chi(\tau;0,z),P(\tau))d\tau}, \\ \mathcal{U}_\phi(z,t) &= \phi(z)e^{-\int_0^t \mu(\chi(\tau;z,0),P(\tau))d\tau}. \end{aligned} \tag{2.9}$$

Now we can derive a system of integral equations in P and B, respectively by integrating (2.8) and β times this equation, in the variable x, $x \in [0,1]$:

$$\begin{cases} P(t) = \displaystyle\int_0^{\sigma(t)} \mathcal{U}_B\big(\theta(0;s,t),t\big)\,ds + \int_{\sigma(t)}^1 \mathcal{U}_\phi\big(\chi(0;s,t),t\big)\,ds, \\ \\ B(t) = \displaystyle\int_0^{\sigma(t)} \beta\big(s,P(t)\big)\,\mathcal{U}_B\big(\theta(0;s,t),t\big)\,ds + \int_{\sigma(t)}^1 \beta\big(s,P(t)\big)\,\mathcal{U}_\phi\big(\chi(0;s,t),t\big)\,ds. \end{cases} \tag{2.10}$$

Let us introduce the following variables:

$$w = \theta(0;s,t) = t + \int_s^0 \frac{1}{g(q)}dq$$

in the first integral of each equation in (2.10), and

$$v = \chi(0;s,t)$$

in the second integral of each equation in (2.10). Note that the range of w is from t to 0, and that of v from 0 to $\chi(0;1,t)$.

Obviously, $dw = -\frac{ds}{g(s)}$ and $s = \chi(t;0,w)$, i.e. $ds = -g(\chi(t;0,w))dw$. Also, for a given fixed t, since $t = \int_v^s \frac{1}{g(q)}dq$ and $s = \chi(t;v,0)$, we have $ds = \frac{g(\chi(t;v,0))}{g(v)}\,dv$.

Thus, the integral equations (2.10) can be written as

$$\begin{cases} P(t) = \displaystyle\int_0^t \mathcal{U}_B(w,t) g(\chi(t;0,w))\, dw + \int_0^{\chi(0;1,t)} \mathcal{U}_\phi(v,t)\, \frac{g(\chi(t;v,0))}{g(v)}\, dv, \\ \\ B(t) = \displaystyle\int_0^t \beta(\chi(t;0,w),P(t)) \mathcal{U}_B(w,t) g(\chi(t;0,w))\, dw + \\ \qquad\qquad \displaystyle\int_0^{\chi(0;1,t)} \beta(\chi(t;v,0),P(t)) \mathcal{U}_\phi(v,t)\, \frac{g(\chi(t;v,0))}{g(v)}\, dv. \end{cases} \tag{2.11}$$

Now, let us substitute (2.9) back into (2.11) to obtain

$$\begin{cases} P(t) = \displaystyle\int_0^t B(w) e^{-\int_w^t \mu(\chi(\tau;0,w),P(\tau))\, d\tau} g(\chi(t;0,w))\, dw + \\ \qquad \displaystyle\int_0^{\chi(0;1,t)} \phi(v) e^{-\int_0^t \mu(\chi(\tau;v,0),P(\tau))\, d\tau}\, \frac{g(\chi(t;v,0))}{g(v)}\, dv, \\ \\ B(t) = \displaystyle\int_0^t \beta(\chi(t;0,w),P(t)) B(w) e^{-\int_w^t \mu(\chi(\tau;0,w),P(\tau))\, d\tau} g(\chi(t;0,w))\, dw + \\ \qquad \displaystyle\int_0^{\chi(0;1,t)} \beta(\chi(t;v,0),P(t)) \phi(v) e^{-\int_0^t \mu(\chi(\tau;v,0),P(\tau))\, d\tau}\, \frac{g(\chi(t;v,0))}{g(v)}\, dv. \end{cases} \tag{2.12}$$

The value of $\chi(0;1,t)$ is well defined if $g(1) \neq 0$. Otherwise, we assume that $\chi(0;1,t) = 1$ and that $\phi(1) = 0$ as was mentioned in the beginning of this section. This last assumption ensures the convergence of the second integrals in each equation of (2.12).

Therefore, if $u(x,t)$ is a solution to the size-structured problem (2.1), then $P(t)$ and $B(t)$ satisfy (2.12). Conversely, if $P(t)$ and $B(t)$ are solutions of (2.12), then it is easy to check that $u(x,t)$ given by (2.5) is a solution to (2.1). The existence of a unique solution of (2.1) or, equivalently, (2.12), is established, for example, in [3], [9].

Selecting $N \in \mathbb{N}$ to represent the number of time steps we want to take, our idea is to approximate $P(t)$ and $B(t)$ for $t = t_i = ih$, $0 \leq i \leq N$, with a given step-size h so that $NH \geq T$. When the coefficients of the system are sufficiently smooth, this can be done with an order of accuracy s as high as desired, provided that the right quadrature formulae are

chosen, that the ordinary differential equation for the characteristic curves is solved with the same accuracy, and that one takes care of choosing with this same accuracy the initial values $P(t_i),\ B(t_i),\ 0 \le i \le k$, where the value of k depends on the order of accuracy s (more details will be given in Section 4).

3 The Case of Linear Death Rates

If μ is a function of size only, i.e. $\mu = \mu(x)$ (the birth rate β may still be nonlinear), the numerical approximation problem becomes considerably easier. In such a case (2.12) becomes a system of Volterra integral equations of the second kind and of the form

$$\begin{cases} X(t) = \displaystyle\int_0^t Y(w)\, K(w,t)\, dw + V(t), \\ \\ Y(t) = \displaystyle\int_0^t Y(w)\kappa\big(w,t,X(t)\big)\, K(w,t)\, dw + U(t,X(t)), \end{cases} \tag{3.1}$$

where $K(w,t) = g(\chi(t;0,w))e^{-\int_w^t \mu(\chi(\tau;0,w))d\tau}$, $\kappa(w,t,P) = \beta(\chi(t;0,w),P)$ and V and U are the second integrals in the two equations of (2.12).

We shall outline now a method to find an approximate solution of a system of the type (3.1) with global error of the order $O(h^4)$. In principle, similar algorithms with higher order of accuracy can be formulated following the same ideas if quadrature rules of higher accuracy are used.

3.1 Some Composite Quadrature Rules

The Newton-Cotes quadrature rules we shall use are of closed and of open type. The former use the values of the integrand function at the end-points of the interval of integration, the latter do not. Suppose that the integral $\displaystyle\int_a^b f(\tau)\, d\tau$ is to be approximated by splitting the

interval $[a,b]=[t_p,t_{p+r}]$ into r subintervals of equal length $h=\frac{b-a}{r}$. The $r+1$ endpoints of those subintervals, $t_{p+j}=a+jh,\ 0\le j\le r$, are called the integration nodes.

Definition 4.1: A family of quadrature formulas $h\sum_{j=0}^{r} q_j^r f(t_{p+j})$ has *order* s if for all sufficiently smooth f the approximation error $E_h(f)=\left|\int_a^b f(t)\,dt - h\sum_{j=0}^{r} q_j^r f(t_{p+j})\right|$ satisfies $E_h(f)=O(h^s)$ as $h\to 0$. We denote

$$\mathcal{Q}_h^s[f;p,r]=h\sum_{j=0}^{r} q_j^r f(t_{p+j}). \tag{3.2}$$

The numbers s and r are not arbitrary, there is a minimum value for r, so that the desired order of accuracy can be attained. For example, if $s=5$, the value of r can be 2, 3, 4 or 5. Namely, for $r=2$, this is Simpson's rule (closed formula),

$$\mathcal{Q}_h^5[f;p,2]=\frac{h}{3}\left[f(t_p)+4f(t_{p+1})+f(t_{p+2}\right]=\int_{t_p}^{t_{p+2}} f(x)\,dx+\frac{1}{90}f^{(4)}(\xi)h^5. \tag{3.3}$$

If $r=3$, this is the closed formula

$$\mathcal{Q}_h^5[f;p,3]=\frac{3h}{8}\left[f(t_p)+3f(t_{p+1})+3f(t_{p+2})+f(t_{p+3})\right]=\int_{t_p}^{t_{p+3}} f(x)\,dx+\frac{3}{80}f^{(4)}(\xi)h^5. \tag{3.4}$$

For $r=4$, this is the open formula

$$\mathcal{Q}_h^5[f;p,4]=\frac{4h}{3}\left[2f(t_{p+1})-f(t_{p+2})+2f(t_{p+3})\right]=\int_{t_p}^{t_{p+4}} f(x)\,dx-\frac{28}{90}f^{(4)}(\xi)h^5 \tag{3.5}$$

Finally, if $r=5$, we have the open formula

$$\begin{aligned}\mathcal{Q}_h^5[f;p,5]&=\frac{5h}{24}\left[11f(t_{p+1})+f(t_{p+2})+f(t_{p+3})+11f(t_{p+4})\right]\\ &=\int_{t_p}^{t_{p+5}} f(x)\,dx-\frac{95}{144}f^{(4)}(\xi)h^5\end{aligned} \tag{3.6}$$

If $r > 5$, the order of accuracy is higher than 5. If $s = 7$, then r can be 4, 5, 6 or 7, i.e. given s, $r = s-3, s-2, s-1, s$; see [8].

Note that the remainder term that gives the accuracy of each formula is of the form $Cf^{(k)}(\xi)h^s$, for some $\xi \in (a, b)$ and has a smaller constant C for closed-type formulae than for the comparable open-type ones.

Composite Newton-Cotes quadrature rules are formed by splitting the interval of integration $[0, t_j]$ into j subintervals of equal length h, then representing j as a sum $j = r_1 + ... + r_\sigma$ and using on each interval of length $r_l h$ a quadrature formula with $r_l + 1$ integration nodes.

Given that closed-type formulae introduce smaller errors than corresponding open-type ones, we want to use a composite quadrature formula formed of just one open-type formula applied on the last subinterval and only closed-type formulae on the other subintervals, all quadratures having the same accuracy $O(h^s)$.

3.2 A Newton-Cotes Numerical Method with Local Error $O(h^5)$

Let us consider the system (3.1) for $(x, t) \in \mathcal{S}$. Assume that for each x and w, $X(\cdot), Y(\cdot), K(x, \cdot)$, $\kappa(x, \cdot, w) \in C^4(0, T)$. Let $h = \frac{1}{M}$ be a given step-size. Denote $t_i = ih, X(t_i) = X_i, Y(t_i) = Y_i$, for $0 \leq i \leq N$, where $Nh \geq T$. Also, denote $w_l = lh, K(w_l, t_i) = K_i^l, \kappa(w_l, t_i, X_i) = \kappa_i^l$.

Consider a fixed time $t = t_n$, $n \geq 6$. We shall use a quadrature formula with 5 nodes (open type) on the interval $[t_{n-4}, t_n]$ and composite quadratures, each with 3 or 4 nodes (closed type) on the interval $[0, t_{n-4}]$ to approximate the integrals in (3.1). It is easy to see that if $n \geq 6$, combinations of closed formulae with 3 or 4 nodes can be used to construct composite rules with accuracy $O(h^5)$. On the other hand, for $n = 5$ a composite formula that includes one open type rule (with 5 nodes) is not possible with accuracy $O(h^5)$. We

insist on using an open-type rule on the final subinterval because in this way the calculation of the approximate solutions of (3.1) is explicit. To formulate an explicit method, we need to approximate the unknowns $X_i, Y_i,\ 0 \le i \le 5$, with accuracy $O(h^5)$ using a procedure called *initialization* that is described in Section 3.4.

For now we shall assume that X_i and Y_i, $0 \le i \le 5$, are known with accuracy $O(h^5)$. Let $\tilde{X}_i, \tilde{Y}_i,\ 0 \le i \le 5$, be approximate values such that

$$\max_{0\le i\le 5} \Big\{ |X_i - \tilde{X}_i|, |Y_i - \tilde{Y}_i| \Big\} < C_1 h^5. \tag{3.7}$$

Since $K(x,t), V(t)$ are known functions, independent of X and Y, $K(lh, ih)$ and $V(ih)$ can be approximated with fifth-order accuracy:

$$\max_{0\le i\le l\le N} \left\{ \left| K(lh,ih) - \tilde{K}_i^l \right|,\ \left| V(ih) - \tilde{V}_i \right|,\ \right\} < C_2 h^5. \tag{3.8}$$

Also, whenever $\tilde{X}_i,\ 0 \le l \le i$ is known, $\kappa(lh, ih, \tilde{X}_i)$ and $U(ih, \tilde{X}_i)$ can be approximated as $\tilde{\kappa}_i^l[\tilde{X}_i]$ and $\tilde{U}_i$ with

$$\left| \kappa(lh, ih, \tilde{X}_i) - \tilde{\kappa}_i^l[\tilde{X}_i] \right| < C_2 h^5; \quad |U(ih, \tilde{X}_i) - \tilde{U}_i| < C_2 h^5. \tag{3.9}$$

Since $\kappa(w,t,P) = \beta\big(\chi(t;0,w), P\big)$, it suffices to obtain a fifth-order approximation of $\chi(t;0,w)$ and this can be accomplished, for example, using the fifth-order Runge-Kutta method for the ODE that defines χ,

$$\frac{d\chi(t;0,w)}{g\big(\chi(t;0,w)\big)} = -dw.$$

$X_i, Y_i, \tilde{X}_i, \tilde{Y}_i, \tilde{V}_i, U_i, \tilde{U}_i$ are discrete functions defined on $\mathcal{I} = \{0, 1, ..., N\}$. Also, for each fixed i, and variable l such that $0 \le l \le i$, $K_i^l, \tilde{K}_i^l, \kappa_i^l, \tilde{\kappa}_i^l[\tilde{X}_i]$ are discrete functions defined on $\mathcal{I} = \{0, 1, ..., N\}$.

Let us define a quadrature rule for such functions in a similar way as (3.2). If $\tilde{f}$ is a

discrete function defined on $\mathcal{I}$, then

$$\mathcal{Q}^5[\tilde{f}; p, r] = h \sum_{j=0}^{r} q_j^r \tilde{f}_{p+j}, , \tag{3.10}$$

where $p + r \leq N$ and q_j^r are the same as in (3.3)–(3.5).

We proceed now to define our numerical method by finding approximations $\tilde{X}_i$, of X_i and $\tilde{Y}_i$ of Y_i, $6 \leq i \leq N$, in the following way:

$$\tilde{X}_i = \mathcal{Q}^5[\tilde{Y}\tilde{K}_i; i-4; 4] + \sum_{q=1}^{L_i} \mathcal{Q}^5 \left[\tilde{Y}\tilde{K}_i; \sum_{p=1}^{q-1} m_p; m_q \right] + \tilde{V}_i, \tag{3.11}$$

where m_q takes the values 2 or 3 and $\sum_{q=1}^{L_i} m_q = (i-4)$.

We use this value to calculate

$$\tilde{Y}_i = \mathcal{Q}^5 \left[\tilde{Y}\tilde{\kappa}_i[\tilde{X}_i]\tilde{K}_i; i-4; 4 \right] + \sum_{q=1}^{L_i} \mathcal{Q}^5 \left[\tilde{Y}\tilde{\kappa}_i[\tilde{X}_i]\tilde{K}_i; \sum_{p=1}^{q-1} m_p; m_q \right] + \tilde{U}_i. \tag{3.12}$$

Also, from (3.1) we can write:

$$X_i = \mathcal{Q}^5[YK_i; i-4, 4] + \sum_{q=1}^{L_i} \mathcal{Q}^5[YK_i; \sum_{p=1}^{q-1} m_p, m_q] + V_i + E_i^1(h), \tag{3.13}$$

$$Y_i = \mathcal{Q}^5[Y\kappa_i[X_i]K_i, i-4; 4] + \sum_{q=1}^{L_i} \mathcal{Q}^5[Y\kappa_i[X_i]K_i; \sum_{p=1}^{q-1} m_p, m_q] + U_i + E_i^2(h). \tag{3.14}$$

E_i^1, E_i^2 are the errors from replacing the integrals in (3.1) with quadratures. Since the local error when replacing an integral on an interval with length $2h$ or $3h$ or $4h$ is $O(h^5)$, then

$$|E_i^1(h)| \leq C_3 h^4, \quad |E_i^2(h)| \leq C_3 h^4.$$

One can define many composite formulae of the type (3.11)–(3.12) since even if the representation of n were a unique combination of multiples of 2 and 3 that led to quadrature

rules with 3 or 4 nodes respectively, these rules could be applied in different orders. This is the reason we define the following method.

Method of formation of composite rules:

1. Given $n \geq 6$, we find uniquely $m, l \in \mathbb{N}_0$ such that $n-4 = 2m+3l$: $l = n \bmod(2), m = \frac{n-4-3l}{2} - l$.

2. We then form the composite rule

$$\sum_{i=1}^{m} \mathcal{Q}^5[f; (i-1)2, 2] + \sum_{i=1}^{l} \mathcal{Q}^5[f; 2m + (i-1)3, 3] + \mathcal{Q}^5[f; n-4, 4],$$

i.e. the 3-node quadratures come first, the 4-node quadrature follows and finally, on the last interval of length $4h$, a 5-node open formula is used. If $m = 0$ or $l = 0$, no summation is performed.

3.3 Convergence and Global Error

Let $\psi_i = |X_i - \tilde{X}_i|; \eta_i = |Y_i - \tilde{Y}_i|, i = 0, 1, ..., N$.

For each $n \geq 6$ and $i = n$ we can subtract (3.11) and (3.12) from (3.13) and (3.14) respectively and bound the differences as follows:

$$\psi_n \leq h \sum_{i=6}^{n-1} qC_4\eta_i + C_0h^5 + C_2h^5 + C_3h^4$$

and

$$\eta_n \leq h \sum_{i=6}^{n-1} qC_5\eta_i + h \sum_{i=6}^{n} qC_6\psi_i + C_0h^5 + C_2h^5 + C_3h^4,$$

where $q = \max_{r,i} |q_i^r|$, while C_4, C_5, C_6 are constants incorporating upper limits for X, Y, K, and κ. $C_0 \leq 6qC_1 \max(C_4, C_5, C_6)$ comes from the evaluation of the error in the first (initialized) integration nodes. When n=6 the first summations in each of the above equations are not present.

We can add and manipulate these two inequalities to obtain

$$\psi_n + \eta_n \leq h \sum_{i=6}^{n-1} qC_7(\psi_i + \eta_i) + C_8 h^4, \tag{3.15}$$

where the term $C_8 h^4$ includes all error terms in the previous two inequalities, including the initial conditions. We then use a discrete Gronwall inequality [7], as stated below.

Let $\{z_n\}, \{g_n\}$ and $\{p_n\}$ be real-valued sequences defined for $0 \leq n \leq N$, such that $p_n \geq 0$ for all n. Assume that, for $n = 0, 1, ..., N$,

$$z_n \leq g_n + \sum_{i=0}^{n-1} p_i z_i,$$

and that $g_n \leq g$. Then

$$z_n \leq g \prod_{j=0}^{n-1} (1 + p_j), \ 0 \leq n \leq N.$$

Using the inequality and (3.15), we obtain

$$\psi_n + \eta_n \leq C_8 h^4 (1 + qC_7 h)^{n-6} \leq qC_8 h^4 (1 + qC_7 h)^{N-6} = O(h^4), \tag{3.16}$$

where $C_7 = \max(C_4 + C_5, C_6)$. Therefore, we can formulate the following result.

Theorem 3.1. *The algorithm (3.11)–(3.12) initialized by values $\tilde{X}_i, \tilde{Y}_i$, $0 \leq i \leq 5$, satisfying (3.7), is convergent with global approximation error $O(h^4)$.* ∎

3.4 Initialization

In order to have a fourth-order method, we need to initialize the numerical approximation (3.11)–(3.12) with six time levels, corresponding to $0 \leq n \leq 5$.

The first one, $n = 0$, is defined using locally fifth order quadratures (e.g. Simpson's rule) to approximate $\tilde{X}_0 = V(0)$ and $\tilde{Y}_0 = U(0)$. The evaluation of the functions V and U in each of the initialization steps is done in an analogous way.

The next one, $n = 1$, requires a special procedure that we leave for last.

For $n = 2$ we use Simpson's formula (3.3) in (3.1) to define implicitly $\tilde{X}_2$ and $\tilde{Y}_2$:

$$\begin{cases} \tilde{X}_2 = \dfrac{h}{3}\,\Big[\tilde{Y}_0\,K(0,2h) + 4\tilde{Y}_1\,K(h,2h) + \tilde{Y}_2\,K(2h,2h)\Big] + V(2h), \\ \\ \tilde{Y}_2 = \dfrac{h}{3}\,\Big[\tilde{Y}_0\,\kappa(0,2h,\tilde{X}_2)\,K(0,2h) + 4\tilde{Y}_1\,\kappa(h,2h,\tilde{X}_2)\,K(h,2h) \\ \qquad\qquad + \tilde{Y}_2\,\kappa(2h,2h,\tilde{X}_2)\,K(2h,2h)\Big] + U(2h). \end{cases} \tag{3.17}$$

We solve this system by iteration, initializing the iterates with $\tilde{X}_2^{(0)} = \tilde{X}_1$ and then recursively solving the second equation in (3.18) for $\tilde{Y}_2$,

$$\tilde{Y}_2^{(i+1)} = \frac{h}{3 - h\kappa\big(2h,2h,\tilde{X}_2^{(i)}\big)K(2h,2h)}\,\Big[\tilde{Y}_0\,\kappa\big(0,2h,\tilde{X}_2^{(i)}\big)\,K(0,2h) + 4\tilde{Y}_1\,\kappa\big(h,2h,\tilde{X}_2^{(i)}\big)\,K(h,2h) + \frac{3}{h}\,U(2h)\Big],$$

followed by solving the first one for $\tilde{X}_2$,

$$\tilde{X}_2^{(i+1)} = \frac{h}{3}\,\Big[\tilde{Y}_0\,K(0,2h) + 4\tilde{Y}_1\,K(h,2h) + \tilde{Y}_2^{(i+1)}\,K(2h,2h)\Big] + V(2h).$$

We continue these iterations until the differences between consecutive iterates are smaller than a prescribed tolerance.

For $n = 3$ we use Newton-Cotes closed-type formula (3.4) in (3.1) to define implicitly $\tilde{X}_3$ and $\tilde{Y}_3$:

$$\begin{cases} \tilde{X}_3 = \dfrac{3h}{8}\,\Big[\tilde{Y}_0\,K(0,3h) + 3\tilde{Y}_1\,K(h,3h) + 3\tilde{Y}_2\,K(2h,3h) + \tilde{Y}_3\,K(3h,3h)\Big] + V(3h), \\ \\ \tilde{Y}_3 = \dfrac{3h}{8}\,\Big[\tilde{Y}_0\,\kappa(0,3h,\tilde{X}_3)\,K(0,3h) + 3\tilde{Y}_1\,\kappa(h,3h,\tilde{X}_3)\,K(h,3h) \\ \qquad + 3\tilde{Y}_2\,\kappa(2h,3h,\tilde{X}_3)\,K(2h,3h) + \tilde{Y}_3\,\kappa(3h,3h,\tilde{X}_3)\,K(3h,3h)\Big] + U(3h). \end{cases} \tag{3.18}$$

We solve this system by iteration, in an entirely analogous way as done for $n = 2$.

For $n = 4$ and $n = 5$ we use the Newton-Cotes formulas of open type (3.5) and (3.6) respectively.

We finally describe the initialization for $t = h$. First, we construct on the time interval $[0, h]$ two quartic polynomials $p(t)$ and $q(t)$ which are fourth order approximations of $X(t)$ and $Y(t)$ respectively on this interval. For example, p can be chosen as the McLaurin polynomial of fourth degree for X and q as the one for Y. Let

$$p(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4, \qquad q(t) = b_0 + b_1 t + b_2 t^2 + b_3 t^3 + b_4 t^4. \tag{3.19}$$

Next we differentiate (3.1) with respect to t to obtain

$$X'(t) = K(w,t)Y(t) + \int_0^t Y(w)\,\frac{\partial K(w,t)}{\partial t}\,dw + V'(t), \tag{3.20}$$

$$\begin{aligned} Y'(t) = \int_0^t Y(w) \left[\frac{\partial \kappa\big(w,t,X(t)\big)}{\partial t} + \frac{\partial \kappa\big(w,t,X(t)\big)}{\partial X} X'(t)\right] K(w,t)\,dw + U'(t) \\ + \int_0^t Y(w)\kappa\big(w,t,X(t)\big)\,\frac{\partial K(w,t)}{\partial t}\,dw + \kappa\big(w,t,X(t)\big)\,K(w,t)\,Y(t). \end{aligned} \tag{3.21}$$

Substituting (3.19) into (3.20)–(3.21), we are led to the equations

$$\begin{cases} p'(t) = K(w,t)q(t) + \displaystyle\int_0^t q(w)\,\frac{\partial K(w,t)}{\partial t}\,dw + V'(t), \\ \\ q'(t) = \displaystyle\int_0^t q(w) \left[\frac{\partial \kappa\big(w,t,p(t)\big)}{\partial t} + \frac{\partial \kappa\big(w,t,p(t)\big)}{\partial X} p'(t)\right] K(w,t)\,dw + U'(t) \\ \qquad\qquad + \displaystyle\int_0^t q(w)\kappa\big(w,t,p(t)\big)\,\frac{\partial K(w,t)}{\partial t}\,dw + \kappa\big(w,t,p(t)\big)\,K(w,t)\,q(t). \end{cases} \tag{3.22}$$

Now we evaluate (3.1) with p in place of X and q in place of Y, for $t = 0$, $t = \frac{h}{2}$, and $t = h$, and we also evaluate (3.22) for $t = 0$ and $t = h$. The integrals in these equations are approximated using Simpson's rule, in order to ensure a fifth-order approximation. The evaluations at $t = 0$ lead to $a_0 = X(0) = V(0)$, $b_0 = Y(0) = U\big(0, X(0)\big)$, $a_1 = X'(0) = K(w,0)b_0 + V'(0)$ and $b_1 = Y'(0) = U'(0) + \kappa\big(w,0,X(0)\big)K(w,0)b_0$. The remaining relations lead to a linear

algebraic system of six equations in six unknowns, the coefficients a_i and b_i, $2 \le i \le 4$, of p and q. The system may or may not have a unique solution. If it does, we finally evaluate (3.19) at $t = h$ for the desired fifth-order approximations

$$\tilde{X}_1 = p(h), \qquad \tilde{Y}_1 = q(h).$$

Alternatively, when the system does not have a a unique solution, we define the remaining Taylor coefficients at $t = 0$ by further differentiation of (3.20) and (3.21), and use the relations $a_i = \dfrac{X^{(i)}(0)}{i!}$ and $b_i = \dfrac{Y^{(i)}(0)}{i!}$, $2 \le i \le 4$.

3.5 The Algorithm for Linear-Death-Rate Size-Structured Equations

In order to have an explicit method fully defined, we need to find $\chi(ih; 0, lh), \chi(ih; lh, 0)$ to be used in (2.12) to write these equations in the form (3.1) with local discretization error of the same order as that used for the numerical quadratures.

For the model described, this amounts to solving ordinary differential equations with local fifth-order accuracy, for example using Runge-Kutta's method.

Remark: If the mortality rate μ depends on the solution—i.e. when we have a nonlinear death rate—it is necessary to find $\int_0^{t_n} F\big(Y(s)\big)\, ds,\ n = 1, 2, 3$, with accuracy $O(h^5)$, where supposedly we only know approximations to $Y(0), Y(h), Y(2h)$. Such an approximation can be found by extrapolation methods [15] but the resulting method is considerably more complicated and will be described and analyzed elsewhere.

4 Conclusions

We presented the classical formulation of size-structured population models in terms of partial differential equations and an equivalent formulation in terms of a system of integral

equations that, in the case of linear mortality rates reduces to a Volterra system of second kind.

We then proposed numerical methods for the approximation of the solution of the last system by quadratures, specifically describing a fourth-order method based on Newton-Cotes formulas. Except for the initialization—that requires the use of an open-type formula based on six nodes—the method described uses exactly one Newton-Cotes formula of open-type based on five nodes (for the last five) coupled with closed-types Newton-Cotes formulas based on three or four nodes.

The initialization of numerical methods originating within this framework will necessarily be quite involved—as the example provided shows—since it always requires approximations at more points than are typically obtained by Newton-Cotes quadrature formulas of the order needed for the given method.

The general framework described and analyzed can provide several other numerical methods, of higher order of convergence if so desired, provided the solution of the differential problem is regular enough. However, the problem of establishing the regularity of the solution of the model in general is still open.

The case of mortality rates that depend on the total population result in considerably more complicated equations that make it impossible to define numerical methods that are explicit in the unknowns. The numerical solution of the problem in such cases will be addressed in a forthcoming paper.

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