J. theor. Biol. (2000) **207**, 217–230
doi:10.1006/jtbi.2000.2168, available online at http://www.idealibrary.com on IDEAL®

Numerical Methods and Parameter Estimation of a Structured Population Model with Discrete Events in the Life History

F. D. L. KELPIN*, M. A. KIRKILIONIS† AND B. W. KOOI*‡

**Faculty of Biology, Free University, De Boelelaan* 1087, 1081 *HV Amsterdam, The Netherlands and*
†Department of Mathematics, Utrecht University, P.O. Box 80010, 3508 *TA Utrecht, The Netherlands*

(*Received on* 25 *January* 1999, *Accepted in revised form on* 9 *August* 2000)

We consider two numerical methods for the solution of a physiologically structured population (PSP) model with multiple life stages and discrete event reproduction. The model describes the dynamic behaviour of a predator–prey system consisting of rotifers predating on algae. The nitrate limited algal prey population is modelled unstructured and described by an ordinary differential equation (ODE). The formulation of the rotifer dynamics is based on a simple physiological model for their two life stages, the egg and the adult stage. An egg is produced when an energy buffer reaches a threshold value. The governing equations are coupled partial differential equations (PDE) with initial and boundary conditions. The population models together with the equation for the dynamics of the nutrient result in a chemostat model. Experimental data are used to estimate the model parameters. The results obtained with the explicit finite difference (FD) technique compare well with those of the Escalator Boxcar Train (EBT) method. This justifies the use of the fast FD method for the parameter estimation, a procedure which involves repeated solution of the model equations.

1. Introduction

We study the transient dynamics of a population of rotifers living in a chemostat after a perturbation from the steady state. The rotifers predate on algae. The algae feed on nitrate which is fed into the chemostat reactor at a constant rate. The reactor is exposed to a sufficient amount of light, so that the algal growth is limited by the amount of nitrate present in the chemostat. The algal and rotifer parameter values are estimated from the experimental data published by Boraas (1993), who performed two consecutive so-called single-stage chemostat experiments on a mixed culture of the algae *Chlorella pyrenoidosa* and the rotifer *Brachionus calyciflorus*. In the first experiment, the nitrate density was changed stepwise and the return of the system to its steady state was monitored. Then, in the second experiment, the algal density was changed and again the transient dynamics were monitored. The algal and rotifer cultures were identical to those used in the two-stage chemostat experiment described in Boraas (1983) and analysed in Kooijman *et al.* (1996) and Kooi & Kooijman (1997, 1999).

The dynamics of the rotifer population is studied using the individual-based population modelling approach. The behaviour of an individual depends both on its own physiological state and on the environmental conditions it experiences. Even under environmentally identical conditions, individuals in the same population need not behave identically if their physiological

‡Author to whom correspondence should be addressed.
E-mail: kooi@bio.vu.nl

0022-5193/00/220217 + 14 $35.00/0

states are different. Physiologically structured population models as described in Metz & Diekmann (1986) and de Roos (1997) allow for differences in the physiological states of the individuals which are represented by the individual's *i-state*. Likely candidates for the *i*-state variables are age, size and energy reserves. The *i*-states of all individuals in a population are summarized in the so-called *p-state*.

An individual's *i*-state may change with time. Continuous changes, for instance growth, are generally described in terms of an ODE. Its solution forms the trajectory followed by the individual in the *i*-state space. Birth, death or some other event, like the hatching of an egg, involves the creation or removal of an individual or a discontinuous jump of its *i*-state. The ODE is defined in each time interval between two successive events. The description of an event matches the final condition for a time interval to the initial condition for the next interval.

The ODEs together with the description of the events form the model for the individual. From this model we derive the model for the dynamics of the *p*-state, usually yielding a set of PDEs. In this article, we study the numerical solution of these *p*-state dynamics. We concentrate on the implementation of the threshold conditions for discrete events.

Two numerical methods are used to simulate the dynamics of a particular rotifer population. One is a simple explicit finite difference (FD) scheme and the other is based on the Escalator Boxcar Train (EBT) package (de Roos, 1996). Comparison of the results obtained with these two techniques facilitates a check on the correctness and performance of the methods. The results of both numerical methods are sufficiently close for the experiment studied.

In these numerical techniques, similar individuals are lumped into cohorts and the dynamics of these cohorts are again described by the sets of ODEs defined at successive time intervals between the events. When these discrete events occur, the number of these ODEs can change or the *p*-state variable can be discontinuous.

The estimates of parameters are calculated by weighted nonlinear regression (Marquardt) of the numerical solutions using experimental data. This procedure may involve many thousands of simulations of the model and therefore requires a time-efficient algorithm. Since the FD scheme is faster it was used in the parameter estimation technique.

A special version of the Dynamic Energy Budget (DEB) model developed by Kooijman (2000) is used to describe the individual rotifer dynamics, i.e. the energy uptake and use for growth and reproduction. The need for a structured modelling approach arises from the propagation mode of the rotifers. They produce eggs. In contrast, algae propagate by fission. Under simplifying assumptions a structured population dynamic model describing them can be reduced to an equivalent unstructured ODE model (Metz & Diekmann, 1989). In this paper, we will make this assumption and treat the algae as an unstructured resource for the rotifers.

The resulting physiologically structured population model, coupled with an unstructured resource, is different from classical models of this type. In contrast to, for example, the McKendrick–von Foerster linear equations (McKendrick, 1929; von Foerster, 1959) or the Gurtin & MacCamy (1974) nonlinear equations, the rotifer model does not assume that every adult individual continuously contributes some kind of effort (fractions of new offspring, energy reserves, etc.) to a common pool from which new offspring are continuously created in time. Mathematically, such a common continuous reproduction pool (modelled as an integral boundary condition for the influx of new offspring) has the property to smooth out discontinuities. The model presented here, similar to other cell-population models, does not share this property. Birth of new individuals occurs when some threshold is reached, that is, birth is modelled here as an event which occurs at discrete times. In Kooi & Kooijman (1997) and Kooi & Kooijman (1999) both propagation modes, continuous vs. discrete, were studied.

2. The Chemostat Model

We introduce subindices for the state variables and the vital parameters to indicate the trophic level: index $i = 0$ denotes the nitrate level, $i = 1$ the algae and $i = 2$ the rotifers. When two population levels are involved in the definition of

TABLE 1

List of symbols. The symbols in the column labeled "dimension" stand for: t time, e energy, l length (of environment) and L length (of organism)

Symbol	Dimension	Interpretation
a, a_b, a_A	t	Age; egg development time; production time
D	t^{-1}	Dilution rate
d_{ve}	—	Conversion factor from structural volume to energy volume
e_b	eL^{-3}	Energy reserve density of eggs at birth
e_E, e_A	eL^{-3}	Energy reserve density of eggs; adults
e_R	eL^{-3}	Energy density for reproduction
$f_{i-1,i}$	—	Scaled functional response: $f_{i-1,i} = x_{i-1}/(k_{i-1,i} + x_{i-1})$
g_i, g_+	—	Energy investment ratio; $g_+ = g_2 + \frac{3}{4}g_2 m_2/v_{1,2}$
$I_{i-1,i}$	$L^3 L^{-3} t^{-1}$	Maximum ingestion rate
$k_{i-1,i}$	$L^3 l^{-3}$	Saturation coefficient
m_i	t^{-1}	Maintenance rate coefficient
p_E	$\#t^{-1}e^{-1}$	Density of eggs
p_A	$\#e^{-2}$	Density of adults
t	t	Time
v, v_b	L^3	Structural volume of individual; birth
x_r	$L^3 l^{-3}$	Nitrate density in the input
x_0	$L^3 l^{-3}$	Nutrient or food density
x_1	$L^3 l^{-3}$	Structural volume density of algae
x_2	$L^3 l^{-3}$	Structural volume density of rotifers
x_E, x_A	$L^3 l^{-3}$	Structural volume density of eggs; adults
$\mu_{i-1,i}$	t^{-1}	Maximum population growth rate
$v_{i-1,i}$	t^{-1}	Specific-energy conductance, $\propto$ assimilation rate

a parameter, two sub-indices will be used. The scaled Holling type II functional responses are defined by $f_{i-1,i} = x_{i-1}/(k_{i-1,i} + x_{i-1})$, where $k_{i-1,i}$ is the saturation constant. Parameter $I_{i-1,i}$ denotes the maximum ingestion rate of the algae and rotifers for $i = 1, 2$, respectively. $\mu_{0,1}$ is the nitrate-limited maximum growth rate of the algae, x_0 denotes the nitrate concentration in the chemostat, and x_1 the algal biovolume (see Table 1 for a list of parameters). The control parameters of the chemostat are the dilution rate, D, and the nitrate concentration in the input, x_r. The model for the nitrate and algae reads

$$\frac{dx_0}{dt} = (x_r - x_0)D - I_{0,1} f_{0,1}(x_0) x_1, \qquad (1)$$

$$\frac{dx_1}{dt} = (\mu_{0,1} f_{0,1}(x_0) - m_1 - D)x_1 - I_{1,2} f_{1,2}(x_1) x_A. \qquad (2)$$

The last term in eqn (2) is the consumption rate of the adult rotifers in the reactor where x_A is the structural volume of the adult rotifers [a precise definition is given in eqn (C.1)]. In the next section, the population model for rotifers is derived.

3. A Physiologically Structured Population Model for Rotifers

The individual model recognizes two stages in the life history of individuals: egg and adult. Upon hatching, eggs become adults and start allocating energy for the use of reproduction. We restrict ourselves to considering rotifer initial conditions that are continuous, with respect to age, as in the experiments by Boraas. Figure 1 gives a graphical representation of the life history of an individual in steady state. The model for the individual rotifers is given in detail in Appendix A. Here the population model is described.

3.1. GRADUAL DEVELOPMENT: FIELD EQUATIONS

3.1.1. *Eggs*

The i-state of the egg consists of two state variables. These are the energy reserve density at

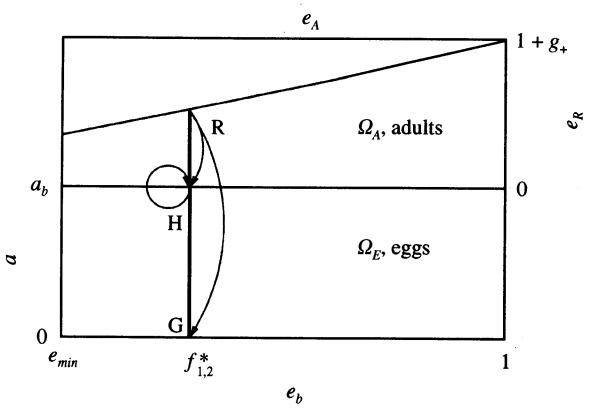

FIG. 1. The trajectory of a rotifer through in the *i*-state space under steady state conditions $e_b = e_A = f^*_{1,2}$. The lower half is the *i*-state space for the eggs $\Omega_E = [e_{min}, 1] \times [0, a_b]$ and the upper half is the *i*-state space for the adults: $\Omega_A = \{(e_A, e_R) | e_{min} \leqslant e_A \leqslant 1 \wedge 0 \leqslant e_R \leqslant e_A + g_+\}$. *G* marks the point of gametogenesis, H the point of hatching and R the reproduction event.

birth $e_b(t) \in [e_{min}, 1]$ and the age $a(t) \in [0, a_b]$. The *i*-state space for the eggs $\Omega_E = [e_{min}, 1] \times [0, a_b]$ is shown in Fig. 1. Here e_{min} is the minimum energy reserve density required to pay the maintenance costs, that is for $e_A < e_{min}$ the individual dies.

The ODEs together with the initial conditions describing the egg development are:

$$\frac{de_b}{dt} = 0, \quad e_b(t_0) = e_A(t_0), \tag{3a}$$

$$\frac{da}{dt} = 1, \quad a(t_0) = 0, \tag{3b}$$

with t_0 the time of gametogenesis and $e_A(t_0)$ the energy reserve density of the mother at this time. These equations describe the trajectory followed by each individual in the *i*-state space. The egg hatches when $a(t) = a_b$, the fixed age at birth. The energy density $e_b + g_+$ is supplied by the mother at gametogenesis and this density is diminished by a fixed amount g_+ from gametogenesis until hatching. The energy amount g_+ represents the energy used for growth of the embryo from gametogenesis till hatching. In Appendix A, equivalent growth functions are given for *i*-state variables v and e_E.

Lifting these individual dynamics to the population level in the chemostat environment, yields the following PDE for the *p*-state $p_E(t, e_b, a)$

$$\frac{\partial p_E}{\partial t} + \frac{\partial p_E}{\partial a} = -Dp_E, \tag{4}$$

where D is the constant dilution rate of the chemostat. Along characteristics of this PDE it reduces to the ODE

$$\frac{dp_E}{da} = -Dp_E, \tag{5}$$

where a is now the parameter along the characteristic.

In steady state, a newly laid egg enters the *i*-state space for eggs at point G in Fig. 1. As the egg ages, it moves up along a vertical line until it reaches the boundary $a = a_b$ (the horizontal line). Here (at point H) the egg hatches and enters the *i*-state space for adults which is shown immediately above the *i*-state space for eggs.

3.1.2. *Adults*

Adults possess energy reserves e_A(t) and an energy buffer with energy allocated to reproduction, $e_R(t)$. The initial energy reserve e_A equals e_b at hatching (at point H). The reproduction buffer is empty at hatching or after the production of an egg and is filled with energy from the energy reserves after payment of energy for maintenance requirements. When this buffer reaches a certain threshold $e_R(t) = e_A(t) + g_+$ (the skew line), the adult produces an egg (point R) and the buffer is emptied (jumps back to point H) and simultaneously lays an egg at point G. The particular threshold ensures that a newborn adult will have the same energy reserve as its mother had when she laid the egg.

The ODEs with initial conditions for the individual adult are

$$\frac{de_A}{dt} = h_A(f_{1,2}, e_A), \quad e_A(t_b) = e_b, \tag{6a}$$

$$\frac{de_R}{dt} = g_A(e_A), \quad e_R(t_b) = 0, \tag{6b}$$

with t_b the time of birth and $f_{1,2}$ the scaled functional response which depends on the algal density x_1.

The dynamics of the population p-state $p_A(t, e_A, e_R)$ is described by the PDE

$$\frac{\partial p_A}{\partial t} + \frac{\partial h_A p_A}{\partial e_A} + \frac{\partial g_A p_A}{\partial e_R} = -Dp_A. \tag{7}$$

The functions h_A and g_A for the adult-stage are given in Appendix A. Analogous to the previous paragraph, along characteristics the PDE reduces to the ODE

$$\frac{\mathrm{d}p_A}{\mathrm{d}a} = -Dp_A, \tag{8}$$

where age a is again the parameter along the characteristics.

3.2. REPRODUCTION EVENTS: THE BOUNDARY CONDITIONS

The boundary conditions for the two hyperbolic PDEs (4) and (7) read, for all e_b where $p_A(t, e_b, e_b + g_+) > 0$:

$$p_E(t, e_b, 0) = \max[g_A(e_b) - h_A(f_{1,2}(x_1(t)), e_b), 0] \times p_A(t, e_b, e_b + g_+), \tag{9a}$$

$$g_A(e_b)p_A(t, e_b, 0) = \max[g_A(e_b) - h_A(f_{1,2}(x_1(t)), e_b), 0] \times p_A(t, e_b, e_b + g_+) + p_E(t, e_b, a_b). \tag{9b}$$

Because of the two stages there are boundary conditions on the transition interface ($a = a_b$, $e_R = 0$). Equation (9b) is this condition for the transition when the egg hatches and becomes a mature adult. The first term on the right-hand side is the inflow of mothers which lay an egg and empty their reproduction buffer. The second term are the hatching eggs, which become adult.

3.3. STEADY STATE: INITIAL CONDITIONS

In the steady state, the amount of algae is constant. The rotifers experience a constant environment. Our particular choice for the reproduction event, that adults lay eggs that will be born with the same energy reserve density that the adults currently have, results in a rotifer population concentrated on one single line in the i-state space.

In the experiments we study, the rotifers are initially in their equilibrium state. There will at all times be only a finite number of states of birth and the population will remain concentrated on lines in the i-state space. On these lines, the p-state can be given as a continuous density function of age as in the method proposed by Murphy (1983).

The initial conditions for the chemostat model, $x_0(0)$, $x_1(0)$, $p_E(0, e_b, a)$ and $p_A(0, e_A, e_R)$ and therefore $x_A(0)$, are derived in Appendix B.

4. Numerical Methods for Physiologically Structured Population Models

Extensive descriptions of numerical methods for the time integration of structured population models are given in de Roos (1988), Ito *et al.* (1991), Milner & Rabbiolo (1992), Sulsky (1993, 1994) and Gurney & Nisbet (1998).

In full discretization schemes, time and i-state space are discretized simultaneously. An example can be found in Ito *et al.* (1991). In Kooi & Kooijman (1997) a simple explicit finite difference scheme was used to solve the model equations. This scheme is equivalent to a forward Euler scheme in the case of an age-structured formulation. As the grid size in both time and age direction are taken equal, the method is also equivalent to integration along the characteristics with equidistant time steps.

In semi-discretization schemes, initially only the i-state space is discretized. In Gurney & Nisbet (1998) a number of these schemes (upwind difference scheme and central difference scheme) are discussed. The resulting set of ODEs is then further discretized in time using an ODE solver. Similar to the full discretization scheme these methods work with a discrete representation of the density function that features in the PDE formulation of the PSP model.

The EBT method (de Roos, 1988) uses a semi-discretization scheme. In order to discretize the i-state space, individuals with similar i-states are grouped into the so-called cohorts. Each cohort is represented by a delta peak placed in the average i-state of the individuals in the cohort. The height of the peak equals the number of

individuals in the cohort. The p-state is approximated by the sum of these delta peaks.

Figure 2 gives an example of the discretization of a one-dimensional i-state space where the p-state is represented by a continuous density function. The method also works, however, for a higher dimensional i-state space and for p-states given by a measure on the i-state space.

Each individual follows a trajectory through the i-state space, which is a solution of the ODE which describes individual development. The right-hand side of the ODE is a function of the individual's i-state and the environment. Initially, cohorts consist of individuals with nearly identical i-states. If the solutions of the development ODE do not diverge, the individuals in a cohort will stay close in between events. As a consequence, the trajectory starting in the initial average i-state of a cohort will at all times be a good approximation for the i-states of the individuals in that cohort. The death rate on this trajectory will also be a good approximation for the death rates of all individuals in the cohort, as death rates too depend only on i-state and environment.

A treatment of classical type boundary conditions with continuous reproduction by all adult individuals can be found in de Roos (1988). The introduction of one or several special boundary cohorts preserves the order of the numerical integration technique. These boundary cohorts are filled with newborn individuals. Once they are large enough they are transformed into ordinary cohorts.

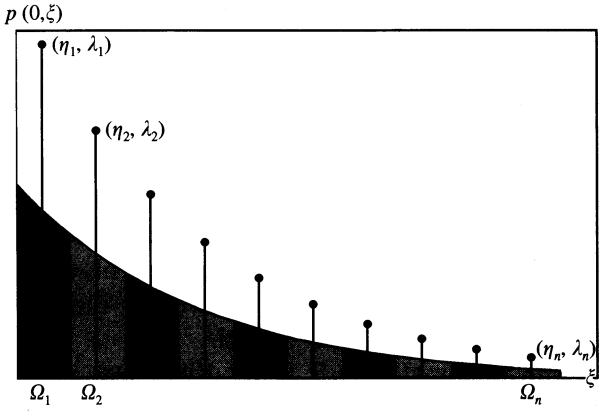

FIG. 2. An i-state discretization of a continuous density function $p(0, \xi)$ into n cohorts. Individuals with i-states in the same range Ω_j form a cohort. This cohort is represented by a delta peak with height $\lambda_j = \int_{\Omega_j} p(0, \xi)\, d\xi$ (the number of individuals in the cohort), placed at $\eta_j = (1/\lambda_j) \int_{\Omega_j} \xi p(0, \xi)\, d\xi$ (the average i-state of all individuals in the cohort).

This discretization of i-state space replaces the p-state PDE of a structured population with a set of ODEs, namely the set which contains for each cohort the development and survival ODEs. If we discretize the i-state spaces of all structured populations in an ecosystem, their ODEs, together with the ODEs for unstructured populations and the environment, form the set of equations to be solved. One may choose from many ODE solvers to solve these systems.

Due to the continuous introduction of new cohorts, the total amount of cohorts may grow so large that the numerical solution of the system is slowed down significantly. If this happens, we can reduce the number of cohorts by merging cohorts with nearly the same i-state or by removing cohorts with a sufficiently small number of individuals.

5. Description of the Two Integration Methods

We consider two numerical realizations for the solution of the equations for the dynamics of the rotifer population with discrete reproduction in the chemostat. Both methods use integration along the characteristics. As described in Section 3, there are two important events in the life of the modelled rotifers. Firstly, the transition from egg to adult and secondly, the reproduction event when the adult lays an egg. In both numerical methods, these two events are treated in a different way. Also the cohorts are merged differently.

5.1. THE FINITE DIFFERENCE SCHEME

A forward-Euler scheme is used to integrate along the characteristic with equidistant time steps both for the eggs and the adults. In Gurney & Nisbet (1998) this method is described for an age-structured model with continuous reproduction. Although this method works with a discrete representation of the density function here we will give a description in terms of cohorts. The number of individuals in a cohort is just the value of the density function in a grid point times the mesh size Δa. For an age-structured model the

characteristics of the PDE are straight 45°-lines in the (a, t)-plane and therefore by taking $\Delta a = \Delta t$ we integrate along the characteristics. This point of view enables us to replace the discretized survival function with the analytical expression for exponential washout with rate D, see also eqns (5) and (8).

One new cohort is created at each time step, which implies that the fixed time step equals the age difference from one cohort to its successor. Having fixed the grid points for the age axis of the eggs, we cannot create new cohorts with arbitrary initial age. We preserve the fixed grid discretizing the age axis by assuming that the new cohort of eggs formed during the past time step, starts with age 0. The development time a_b of the egg is fixed, so we can choose the time step in such a way that the transition from egg to adult occurs at a grid point. This implies that no estimation is needed for the time of hatching.

In contrast, the time of reproduction depends on the environmental conditions. Thus, we cannot choose a fixed time step in such a way that reproduction always occurs exactly at a grid point. We use the two points $e_R(t)$ and $e_R(t + \Delta t)$ to estimate the time $\tau \in [t, t + \Delta t]$ at which $e_R(\tau)$ lies on the boundary. From this estimate, we calculate the amount of energy allocated to reproduction after laying the egg, i.e. in the time interval $[\tau, t + \Delta t]$. We reset the reproduction buffer to this amount and add a new cohort of eggs with age 0 (instead of age $t + \Delta t - \tau$) yielding a small extra discretization error. To prevent rapid increase of the number of cohorts, all newly laid eggs by different reproducing cohorts are lumped into one cohort. The e_b value of this cohort equates the average of the estimated values of $e_A(\tau)$ of all mothers in the different reproducing cohorts. We stress that the scaled energy reserves for all the reproducing adult individuals are almost the same, for $e_A(t)$ of each individual converges exponentially to the scaled functional response $f_{1,2}$. This is a consequence of the first-order kinetics for the energy reserves, eqn (A.2a).

5.2. THE ESCALATOR BOXCAR TRAIN METHOD

The EBT package (de Roos, 1996) features a fourth–fifth order Runge–Kutta–Fehlberg method for the time integration. The boundary cohorts mentioned in Section 4 are not suitable for the implementation of discrete reproduction, because there is no birth rate. Instead, reproduction events are handled using an iterative procedure, already implemented in the EBT package (de Roos, 1996), which iterates the same integration step with different step-sizes Δt until $t + \Delta t$ is sufficiently close to τ. At that time the reproduction buffer of the cohort of mothers is set to zero and a cohort of newborn eggs is added to the population. The transition from egg to adult happens at a fixed age a_b. Therefore, the proper step-size $\Delta t = a_b - a(t)$ can be calculated beforehand.

Each time a cohort of mothers reproduces, a new cohort of eggs is created. Therefore, the number of cohorts increases rapidly beyond bounds and we need to merge appropriate cohorts. All the cohorts are compared at regular time intervals. If two cohorts have got sufficiently close to each other both in the e_A direction and in the e_R direction, they are merged. We used a stricter condition in the e_R direction. The e_A i-state variable of cohorts tends towards $f_{1,2}$ exponentially. As already mentioned above, this means that cohorts get closer to each other in that direction all the time since the difference between the e_A variables decreases exponentially.

Cohorts hatch and reproduce with time intervals of about 15–20 hr. Hence, each cohort generates about 0.06 events per hour and because these events are not synchronized, 1000 cohorts can be expected to generate 60 events per hour. Analysis of simulation runs shows that this indeed happens. Since all individuals compete for a common food source in a homogeneous environment, each event that happens to a single individual influences the dynamics of all individuals. Therefore, we must cease integration whenever an event happens, and the ODE solver cannot use large stepsizes for the time integration. This explains why the EBT method combined with this implementation of the discrete events, is rather slow for this problem.

5.3. ACCURACY OF THE SIMULATIONS

We repeated the calculations with increasing discretization precision in order to assess the

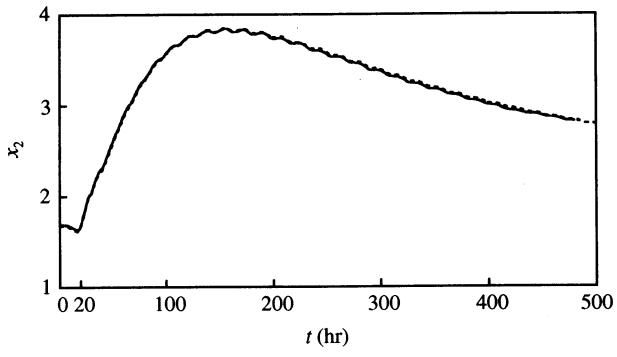

FIG. 3. Simulation results for the rotifer densities in a chemostat after a perturbation from the steady state. (——) represents rotifer biomass calculated with the finite difference technique and (- - -) calculated with the EBT package.

accuracy of the numerical methods. Firstly, starting simulation with the discretized analytical steady-state solution derived in Appendix B with increasing discretization precision we found a decreasing global error for each method separately. Secondly, for each method separately we checked convergence of the simulation results for increasing discretization precision. Thirdly, we compared the simulation results obtained with the two numerical methods. The results are shown in Fig. 3 where we show the structural volume density of rotifers, x_2. Some differences between the two lines can be expected because of the rather crude merging technique in the FD method where all newly laid eggs form one cohort. This difference is small for this experiment and this justifies the use of the faster FD scheme for the parameter estimation procedure described in Section 7.2.

6. Simulation Results

Figure 4 gives an impression of the dynamics of the rotifer population after the algal pulse. These results were obtained with the EBT method. The addition of algae increased $f_{1,2}$ from $f_{1,2}^*$ in Fig. 1, to the value indicated at the bottom of the frame. The eggs only age so they will always move straight up through the i-state space. The adult rotifers' energy density exponentially tends towards $f_{1,2}$ so in the first pictures after the algal pulse all adult cohorts move very quickly to the right. The adults also keep filling their reproduction buffer (e_R), which causes them to move upwards. The pictures illustrate that the population remains concentrated on lines.

The results are shown till $t = 20$ hr. After this period the trajectories in the i-state space "converge" to the situation at $t = 0$, the line $e_b = e_A = f_{1,2}^*$. This is a consequence of the assumption that the energy reserves supplied by the mother to the egg are such that at hatching the energy density of the newborn adult equates that of the mother at the instant the mother lays the egg.

Since for finite time the number of generations is finite, the distribution with respect to the energy reserves (for eggs, e_b, and adults, e_A), that is for fixed age, a, is described by a superposition of a finite number of δ-functions.

Observe the rather sharp bend in the structural volume density of rotifers, x_2, in Fig. 3 for $t \approx 20$. Figure 4 shows that for a small period after $0 \leqslant t \lesssim 6$ there is no reproduction. No adult reaches the threshold value for the reproduction buffer because $g_A(e_b) - h_A(f_{1,2}(x_1(t)), e_b) = v_{1,2}(2e_b - f_{1,2}(x_1(t))) < 0$, eqn (A.2), for small values of t since $f_{1,2}(x_1(t))$ is then rather large (see the value of $f_{1,2}$ indicated at the bottom of the frame). This clarifies the decrease of the rotifer density function x_2. From $t \approx 20$ on the rotifer density increases again because the energy reserves e_A are high (due to the algal pulse at $t = 0$) combined with a continuous inflow of newly laid eggs.

7. Comparison of Simulation Results with the Data sets

In this section, we estimate the parameters of the chemostat model formed by the set of ODEs (1) and (2), coupled via x_A with the PDEs (4) and (7) with the boundary conditions (9) and initial conditions $x_0(0)$, $x_1(0)$, $p_E(0, e_b, a)$, $p_A(0, e_A, e_R)$ and $x_A(0)$.

7.1. EXPERIMENTAL DATA

The experiments are described in Boraas (1993). In this single-stage chemostat experiment the dilution rate was $D = 0.0275\,\mathrm{hr}^{-1}$ and the nitrate concentration in the inflow is $x_r = 7\,\mu\mathrm{g\,N\,ml}^{-1}$.

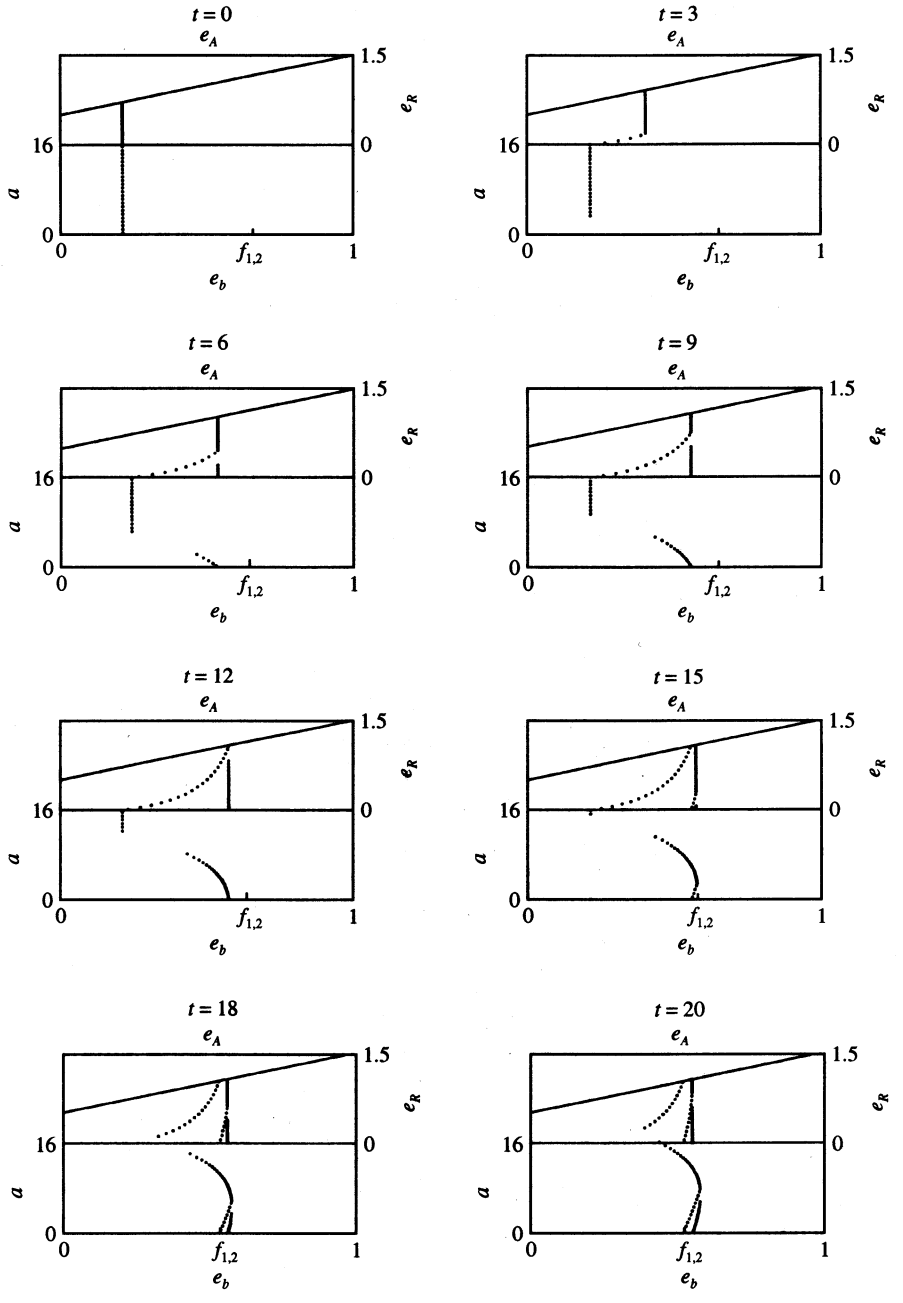

FIG. 4. Snapshots of the average i-states of the cohorts making up the rotifer population during the first 20 hr of the chemostat algal pulse experiment. The lower half is the i-state space for the eggs $\Omega_E = [e_{min}, 1] \times [0, a_b]$ and the upper half is the i-state space for the adults: $\Omega_A = \{(e_A, e_R) | e_{min} \leqslant e_A \leqslant 1 \wedge 0 \leqslant e_R \leqslant e_A + g_+\}$. The horizontal line at $a = a_b = 3/\nu_{1,2} \approx 16$ denotes the transition from egg to adult. The skew line, $e_R = e_A + g_+ \approx 1.5$, denotes the condition for discrete reproduction. These results were obtained with the EBT method. To get a clearer picture, we discretized into 50 cohorts and did not merge cohorts. For an explanation of the figure see Section 5.

The experimental data sets consist of the algal and rotifer population dry-weights as a function of time. We assume a fixed conversion factor for biovolume-to-dry-weight and therefore it suffices to derive expressions for the biovolumes (the sum of the structural and energy components). The conversion factors given in Boraas (1983) are 0.10 and 0.57 $g\,cm^{-3}$ for rotifers and algae, respectively.

In Fig. 5, the time course of the culture before and during a pulse of nitrate is shown. These transient time course data extend from the time

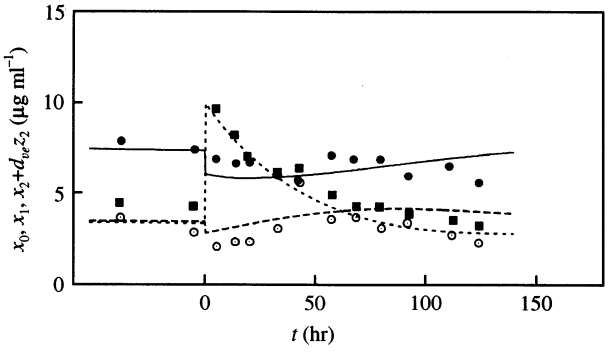

FIG. 5. Experimental data for chemostat nitrate pulse experiment after Boraas (1993). Symbols ●, ⊙ and ■ represent measured rotifer dry-weight density, algal dry-weight density and nitrate concentration, respectively. Simulation results for the response of nitrate, algal and rotifer densities in a chemostat. (——) represents rotifer biomass, $x_2 + d_{ve}z_2$ (μg ml^{-1}), and (– – –) represents algal dry-weight, $x_1(t)$ (μg ml^{-1}), and (- - -) represents nitrate concentration, $x_0(t)$ (μg N ml^{-1}). Values assigned to physiological parameters are listed in Table 2.

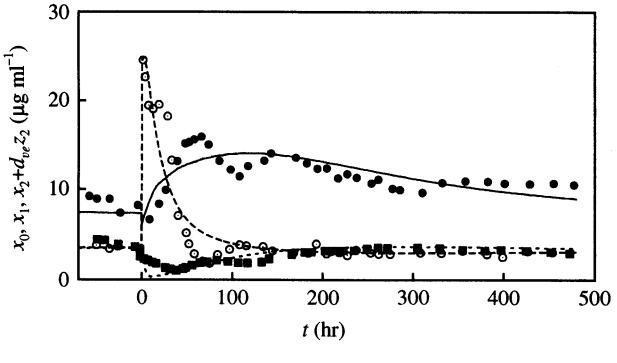

FIG. 6. Experimental data for chemostat algal pulse experiment after Boraas (1993). Symbols ●, ⊙ and ■ represent measured rotifer dry-weight density, algal dry-weight density and nitrate concentration, respectively. Simulation results for the response of nitrate, algal and rotifer densities in a chemostat. (——) represents rotifer biomass, $x_2 + d_{ve}z_2$ (μg ml^{-1}), and (– – –) represents algal dry-weight, $x_1(t)$ (μg ml^{-1}), and (- - -) represents nitrate concentration, $x_0(t)$ (μg N ml^{-1}). Values assigned to physiological parameters are listed in Table 2.

that the three component system (nitrate, algae, rotifers) had been "stable" for ca. 15 days. The transient time course data during and after a pulse of algae is shown in Fig. 6. These data were collected from the same culture immediately after the nitrate pulse shown in Fig. 5. At $t = 0$, a pulse of algae is supplied in the reactor:

> This algal pulse was produced by injecting 100 ml of algal suspension, which was growing in a parallel uni-specific algal chemostat maintained under environmental conditions identical to the mixed-species chemostat. This resulted in approximately an eight-fold increase in the algal concentration in the mixed-species chemostat and a dilution of the nitrate and rotifer concentrations.

Boraas mentioned that the algal steady state value is about 3–4 μg ml^{-1}, so the initial value at $t = 0$ would be 24–32 μg ml^{-1}. The measured peak value is ≈ 25 μg ml^{-1} and therefore we assumed that the algal density was increased to that value. The nitrate and rotifer densities were decreased stepwise by a factor (570 − 100)/570 where 570 ml is the volume of the rotifer vessel (Walz, 1993, p. 23).

7.2. PARAMETER ESTIMATION

The FD scheme is used for parameter estimation with a weighted nonlinear regression (Marquardt) for the algal and rotifer population models. To be able to compare measured data from Boraas (1993) with model predictions we have to give explicit expressions for the structural volume of the adults and eggs and expressions for the contributions of the energy contents to the dry-weight of the rotifer population. In Appendix C, these expressions are given.

In this case, we have ten parameters but during the regression of both data sets simultaneously, one parameter was fixed: $m_2 = 0$. The estimated values are shown in Table 2. Curve fitting with all parameters being free gave a negative maintenance rate coefficient m_2. Because a negative maintenance rate coefficient is unrealistic, we put the constraint $m_2 = 0$, although a positive value would be even more realistic from a biological point of view.

After the nitrate pulse neither the algal nor the rotifer population showed hardly any response. In Fig. 5, the measured time course data for the nitrate–algal–rotifer densities are shown. This suggests that in steady state with $D = 0.0275$ hr^{-1} and $x_r = 7$ μg N ml^{-1}, the hyperbolic functional response $f_{1,2}$ is close to one: stated otherwise, the saturation constant $k_{0,1}$ must be smaller than the steady state value for the nitrate x_0^*. Simultaneous nonlinear regression of both data sets, namely the nitrate and the

TABLE 2

Parameter set for the single-stage chemostat model. The control parameters are the dilution rate $D = 0.0275\,\mathrm{hr}^{-1}$ *and the nitrate concentration in the inflow* $x_r = 7\,\mu\mathrm{g\,N\,ml}^{-1}$. *The maximum growth rate is defined by* $\mu_{i-1,i} = v_{i-1,i}/g_i$. *The egg development time* $a_b = 3/v_{1,2} \approx 16\,\mathrm{hr}$. *Because* $m_2 = 0$ *we have* $e_{min} = 0$ *and* $g_+ = g_2 = 0.502$

Parameter	Values	
	$i = 1$	$i = 2$
$\mu_{i-1,i}$	$0.073\,\mathrm{hr}^{-1}$	—
$k_{i-1,i}$	$0.855\,\mu\mathrm{g\,N\,ml}^{-1}$	$13.016\,\mu\mathrm{g\,ml}^{-1}$
$I_{i-1,i}$	$0.036\,\mu\mathrm{g\,N\,(\mu g\,hr)}^{-1}$	$0.010\,\mathrm{hr}^{-1}$
m_i	$0.029\,\mathrm{hr}^{-1}$	0.0
g_i	∞	0.502
$v_{i-1,i}$	∞	$0.187\,\mathrm{hr}^{-1}$
d_{ve}	—	2.124

algal pulse experiments, gives a realistic value for $k_{0,1}$ which is well below the steady state value mentioned by Boraas: $x_0^* \approx 5\,\mu\mathrm{g\,N\,ml}^{-1}$.

Simulations with the estimated parameter values given in Table 2, result in rather good fits. Unfortunately, the relatively fast oscillations which look very realistic are not captured by the model. When parameters were tuned in such a way that the resulting dynamics shows oscillations with similar frequencies as the measured frequencies, the amplitudes were far off.

8. Discussion and Conclusions

Because of lack of proofs of convergence for both methods we assessed the performance of the numerical methods by simulation. In this paper, we show that the forward Euler finite difference scheme yields acceptable accuracy by comparing the results with a more elaborate semi-discrete EBT approach of de Roos.

The numerical algorithm consists of three parts, namely integration, threshold-passing and merging of cohorts which are mutually dependent. When a first-order time-integration is used, linear interpolation in the threshold-passing and merging of all the newly laid eggs in one cohort are appropriate counterparts. The finite difference method yields a very fast algorithm. The success of the FD method is to some extent related to the specific properties of this case study. The first-order kinetics for the energy reserves ensures that the energy reserves of different reproducing mothers are almost the same. This justifies the lumping of all newborn individuals into a single cohort. For our example it was therefore advantageous not to use a general purpose method like the EBT method for our parameter estimation procedure. It is probably also the case in other computer-intensive tasks such as bifurcation problems where one or several bifurcation parameters are varied and the asymptotic behaviour of the system is studied. This has been discussed in Kirkilionis *et al.* (1997).

To speed up the performance of the EBT method, we can take larger steps for most of the population anyway and take small steps only for those cohorts that hatch or reproduce. If we do this, we need to assume that the influence of the hatching and reproducing cohorts, on the dynamics of the other individuals, during the time from the event to the end of the large time step, is sufficiently small. As the EBT method is used as a reference to check the correctness of the FD method, we refrain from making such assumptions for this method. In Section II.6 of Hairer *et al.* (1987) the construction of the so-called dense output formulas for Runge–Kutta methods is discussed. These techniques, such as the DOPRI method or a Hermite interpolation, can be used for the event location instead of the iterative procedure.

Discrete phenomena in the lifetime of an individual also occur with other species. As an example, we mention the life history of a water-fly which moults at fixed time-intervals. In de Roos *et al.* (1997) the relationship between the *Daphnia pulex* individual behaviour and the dynamics of the population is discussed. Whenever an individual moults, it sheds its carapace, releases its eggs and deposits new eggs in the brood pouch provided it has allocated sufficient energy to produce at least one egg.

Discrete events also occur in cell populations when cells enter different stages of their life cycle. This is relevant in cancer research or when considering detailed phytoplankton dynamics. Efficient algorithms for discontinuous vital rates are therefore relatively important. The proposed numerical techniques can take account of these

discrete processes and additional assumptions, for instance a continuous birth rate at the population level need not be made in advance.

The authors would like to thank Martin Boer, Odo Diekmann, Paul Hanegraaf, Waltraud Huyer, Bas Kooijman, Ben Sommeijer and Cor Zonneveld for valuable discussions. This research was supported by the Netherlands Organization for Scientific Research (NWO) as part of the NWO priority program MPR (Massive Parallel Computing).

REFERENCES

BORAAS, M. E. (1983). Population dynamics of food-limited rotifers in two-stage chemostat culture. *Limnol. Oceanogr.* **28,** 546–563.

BÖRAAS, M. E. (1993). Single-stage predator–prey algal–rotifer chemostat cultures. In: *Plankton Regulation Dynamics* (Walz, N., ed.), Vol. 98, *Ecological Studies*, pp. 51–61. Berlin: Springer-Verlag.

DE ROOS, A. M. (1988). Numerical methods for structured population models: the escalator boxcar train. *Num. Meth. Part. Diff. Eq.* **4,** 173–195.

DE ROOS, A. M. (1996). Escalator boxcar train package (version 2.0). ftp://toranaga.bio.uva.nl/pub/andre/programs/old/escbox-2.0/escbox2.tar.Z.

DE ROOS, A. M. (1997). A gentle introduction to physiologically structured population models. In: *Structured-Population Models in Marine, Terrestrial, and Freshwater Systems* (Tuljapurkar, S. & Caswell, H., eds), pp. 119–204. London: Chapman & Hall.

DE ROOS, A. M., MCCAULEY, E., NISBET, R. M., GURNEY, W. S. C. & MURDOCH, W. W. (1997). What individual life histories can (and cannot) tell about population dynamics. *Aquatic Ecol.* **31,** 37–45.

GURNEY, W. S. C. & NISBET, R. M. (1998). *Ecological Dynamics.* Oxford: Oxford University Press.

GURTIN, M. E. & MACCAMY, R. C. (1974). Nonlinear age-dependent population dynamics. *Arch. Rat. Mech. Anal.* **54,** 281–300.

HAIRER, E., NORSETT, S. & WANNER, G. (1987). *Solving Ordinary Differential Equations I*, Vol. 8, *Springer series in Computational Mathematics.* New York: Springer-Verlag.

ITO, K., KAPPEL, F. & PEICHL, G. (1991). A fully discretized approximation scheme for size-structured population models. *SIAM J. Numer. Anal.* **28,** 923–954.

KIRKILIONIS, M. A., DIEKMANN, O., LISSER, B., NOOL, M., DE ROOS, A. M. & SOMMEIJER, B. P. (1997). Numerical continuation of equilibria of physiologically structured population models I. Theory. Technical Report, CWI-report MAS-R9714, P.O. Box 94079, 1090 GB Amsterdam, The Netherlands.

KOOI, B. W. & KOOIJMAN, S. A. L. M. (1997). Population dynamics of rotifers in chemostats. *Nonlinear Anal. Theory, Methods & Appl.* **30,** 1687–1698.

KOOI, B. W. & KOOIJMAN, S. A. L. M. (1999). Discrete event versus continuous approach to reproduction in structured population dynamics. *Theoret. Popul. Biol.* **56,** 91–105.

KOOIJMAN, S. A. L. M. (2000). *Dynamic Energy and Mass Budgets in Biological Systems.* Cambridge: Cambridge University Press.

KOOIJMAN, S. A. L. M., KOOI, B. W. & BOER, M. P. (1996). Rotifers do it with delay: The behaviour of reproducers vs. dividers in chemostats. *Nonlin. World* **3,** 107–128.

MCKENDRICK, A. G. (1929). Application of mathematics to medical problems. *Proc. Edinb. Mathe. Soc.* **44,** 98–130.

METZ, J. A. J. & DIEKMANN, O. (1986). *The Dynamics of Physiologically Structured Populations*, Vol. 68, *Lecture Notes in Biomathematics.* Berlin: Springer-Verlag.

METZ, J. A. J. & DIEKMANN, O. (1989). Exact finite dimensional representations of models for physiologically structured populations I. In: *Differential Equations with Applications in Biology*, (Goldstein, J. A., Kappel, F. & Schappacher, W., eds). pp. 266–297. Physics and Engineering. New York: Marcel Dekker.

MILNER, F. A. & RABBIOLO, G. (1992). Rapidly converging numerical algorithms for models of population dynamics. *J. Math. Biol.* **30,** 733–754.

MURPHY, L. F. (1983). A nonlinear growth mechanism in size structured population dynamics. *J. theor. Biol.* **104,** 493–506.

SULSKY, D. (1993). Numerical solution of structured population models I: Age structure. *J. Math. Biol.* **31,** 817–839.

SULSKY, D. (1994). Numerical solution of structured population models II: Mass structure. *J. Math. Biol.* **32,** 491–514.

VON FOERSTER, H. (1959). Some remarks on changing populations. In: *The Kinetics of Cellular Proliferation.* (Stohlman, F. ed.). New York: Grune and Stratton.

WALZ, N. (1993). *Plankton Regulation Dynamics*, Vol. 98, *Ecological Studies.* Berlin: Springer-Verlag.

APPENDIX A

Growth Functions for Rotifers

In this appendix, we give the growth function for the individual rotifers. An interpretation of the symbols we use can be found in Table 1. The individual model for the rotifers is a simplified version of the DEB model (Kooijman, 2000). This model recognizes three stages in the life history of individuals: egg, juvenile and adult. Eggs neither eat nor reproduce, juveniles eat but do not reproduce and adults both eat and reproduce. In this study, we ignore the juvenile stage, which is relatively short for rotifers. So upon hatching, eggs immediately become adults and start allocating energy for the use of reproduction. For an extensive discussion and motivation of the model used for the individuals, the reader is referred to Kooijman *et al.* (1996), Kooi & Kooijman (1997, 1999).

A.1. EGGS

The *i*-state of the egg consists of two state variables. These are the structural volume $v(t) \in [0, v_b]$ and the energy reserve density $e_E(t) \in [e_{min} + g_+, 1 + g_+]$. The ODEs describing the

egg development are

$$\frac{dv}{dt} = g_E(v) = v_{1,2} v^{2/3} v_b^{1/3}, \quad v(t_0) = 0, \quad \text{(A.1a)}$$

$$\frac{de_E}{dt} = h_E(v) = -\left(v_{1,2} g_2 \left(\frac{v_b}{v}\right)^{1/3} + m_2 g_2\right)\frac{v}{v_b},$$

$$e_E(t_0) = e_b + g_+, \quad \text{(A.1b)}$$

with t_0 the time of gametogenesis. The egg hatches when $v(t) = v_b$, the fixed size at birth. At this time, the egg has a fixed age a_b and scaled energy reserves e_b. The energy density $e_b + g_+$ is supplied by the mother at gametogenesis and this density is diminished by a fixed amount $g_+ = g_2 + \frac{3}{4} m_2 g_2 / v_{1,2}$ from gametogenesis until hatching.

Change of i-state variables v, e_E to e_b, a gives the equivalent formulation (3a) and (3b).

A.2. ADULTS

Besides their energy reserves $e_A(t)$, adults possess an energy buffer with energy allocated to reproduction, $e_R(t)$.

The ODEs for the individual adult are

$$\frac{de_A}{dt} = h_A(f_{1,2}, e_A) = v_{1,2}(f_{1,2}(t) - e_A),$$

$$e_A(t_b) = e_b, \quad \text{(A.2a)}$$

$$\frac{de_R}{dt} = g_A(e_A) = v_{1,2} e_A - m_2 g_2, \quad e_R(t_b) = 0, \quad \text{(A.2b)}$$

with t_b the time of birth and $f_{1,2}(t)$ the scaled functional response. We assume that $e_A > e_{min} = m_2 g_2 / v_{1,2}$, that is, there is always sufficient energy reserves to "pay" maintenance costs. This is ensured when food is abound.

APPENDIX B

Calculating the Initial Conditions

In both experiments performed by Boraas (1993), the rotifer population is assumed to be in steady state at $t = 0$ when the nitrate or algal density are changed stepwise. A superscript asterisk, *, will indicate the value of a variable in this steady state. The steady state values can be derived from the following equations:

$$\exp\{Da_A^*\} = 1 + \exp\{-Da_b\}, \quad \text{(B.1)}$$

where a_A is the production time of an egg. Its steady state value is

$$a_A^* = \frac{g_+ + f_{1,2}^*}{v_{1,2} f_{1,2}^* - m_2 g_2}. \quad \text{(B.2)}$$

Because $f_{1,2}^* = e_A > e_{min} = m_2 g_2 / v_{1,2}$ this expression is well defined. Equation (B.1) means that the net reproduction of each individual equals one, that is, each adult replaces itself. Subsequently, we find an expression for the functional response $f_{1,2}^*$ in steady state

$$f_{1,2}^* = \frac{\ln\{1 + \exp\{-Da_b\}\} m_2 g_2 / D + g_+}{\ln\{1 + \exp\{-Da_b\}\} v_{1,2} / D - 1}. \quad \text{(B.3)}$$

In steady state the definition of Holling type II functional response gives the biomass density for the algae

$$x_1^* = \frac{k_{1,2} f_{1,2}^*}{1 - f_{1,2}^*}. \quad \text{(B.4)}$$

Setting the right-hand side of eqn (1) equal to zero, we conclude that the nitrate density x_0^* is the positive root of

$$(x_0^*)^2 + \left(\frac{I_{0,1} x_1^*}{D} + k_{0,1} - x_r\right) x_0^* - x_r k_{0,1} = 0. \quad \text{(B.5)}$$

Analogously, the right-hand side of eqn (2) yields

$$x_A^* = \frac{(\mu_{0,1} f_{0,1}^*(x_0^*) - D - m_1) x_1^*}{I_{1,2} f_{1,2}^*}, \quad \text{(B.6)}$$

where of course

$$f_{0,1}^*(x_0^*) = \frac{x_0^*}{k_{0,1} + x_0^*}. \quad \text{(B.7)}$$

We also need the steady p-states $p_E^*(e_b, a)$ and $p_A^*(e_A, e_R)$. These functions are only non-zero for

$e_b = e_A = f^*_{1,2}$ and in those cases they are given by

$$p_E(0, e_b, a) = \delta_{f^*_{1,2}}(e_b) p^*_E(f^*_{1,2}, a)$$

$$= \frac{x^*_A}{v_b} \frac{D \exp\{-C(f^*_{1,2} + g_+)\}}{1 - \exp\{-C(f^*_{1,2} + g_+)\}} \exp\{-Da\}, \quad \text{(B.8a)}$$

$$p_A(0, e_A, e_R) = \delta_{f^*_{1,2}}(e_A) p^*_A(f^*_{1,2}, e_R)$$

$$= \frac{x^*_A}{v_b} \frac{C}{1 - \exp\{-C(f^*_{1,2} + g_+)\}} \exp\{-Ce_R\}, \quad \text{(B.8b)}$$

where $C = D/(v_{1,2} f^*_{1,2} - m_2 g_2)$. Because $f^*_{1,2} = e_A > e_{min} = m_2 g_2 / v_{1,2}$, C is positive.

APPENDIX C

Calculating the Rotifer Population Measured Variables

In this appendix, we give the explicit expressions for the dry-weight of the rotifer population as function of the population density functions.

The rotifer adults do not grow and therefore the relationship between structural volume $x_A(t)$ and density $p_A(t, e_A, e_R)$ is simply

$$x_A(t) = \int_{e_{min}}^{1} \int_0^{e_A + g_+} v_b p_A(t, e_A, e_R) \, de_R \, de_A. \quad \text{(C.1)}$$

For the eggs the structural volume $x_E(t)$ can be derived using $v(a)$ the solution of eqn (A.1a):

$$x_E(t) = \int_{e_{min}}^{1} \int_0^{a_b} v(a) p_E(t, e_b, a) \, da \, de_b. \quad \text{(C.2)}$$

The total structural volume of the rotifer population is taken as $x_2(t) = x_A(t) + x_E(t)$.

The energy-volume of the reserves in the adults, denoted as $z_A(t)$, is defined by

$$z_A(t) = \int_{e_{min}}^{1} \int_0^{e_A + g_+} e_A v_b p_A(t, e_A, e_R) \, de_R \, de_A. \quad \text{(C.3)}$$

The energy-volume allocated to reproduction is defined by

$$z_R(t) = \int_{e_{min}}^{1} \int_0^{e_A + g_+} e_R v_b p_A(t, e_A, e_R) \, de_R \, de_A. \quad \text{(C.4)}$$

The energy-volume of the reserves in the eggs, denoted by $z_E(t)$, is

$$z_E(t) = \int_{e_{min}}^{1} \int_0^{a_b} e_E(e_b, a) v_b p_E(t, e_b, a) \, da \, de_b, \quad \text{(C.5)}$$

where $e_E(e_b, a)$ is the energy reserve of an egg with $e_E = e_b + g_+$ at age $a = 0$ and $e_E = e_b$ at age $a = a_b$. This quantity is given by the solution of eqn (A.2a).

The energy-volume of the rotifer population is given by $z_2(t) = z_A(t) + z_R(t) + z_E(t)$. The total biovolume of the rotifer population is the structural volume plus the energy-volume $x_2(t) + d_{ve} z_2(t)$, where d_{ve} is a conversion factor from structural volume to energy-volume. The reader is referred to Kooijman *et al.* (1996) and Kooi & Kooijman (1997, 1999) for details.