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Monte Carlo simulation program for ecosystems

*Antoni Giró, Joaquim Valls, Joan A.Padró[1] and Jorge Wagensberg[1]**

Abstract

A Monte Carlo computer simulation program is designed in order to describe the spatial and time evolution of a population of living individuals under preassigned environmental conditions of energy. The simulation is inspired by previous techniques developed in physics – in particular, in molecular dynamics and simulations of liquids – and it already provides some new insights regarding macroscopic deterministic models in ecology and concerning eventual control of artificial biomass production plants.

Introduction

The Monte Carlo method is today a well-known technique in statistical mechanics. The simulation of the microscopic behaviour of matter is available for a low population of molecules ($n \leq 1000$) by means of random numbers. The aim of this procedure is the derivation of macroscopic parameters that match with observation. Some recent results in ecological populations (Lurie *et al.*, 1983, Lurie and Wagensberg, 1983) suggested the application of such a simulation tool in order to explore the macroscopic state of an ecological system from its individual characteristics and interactions. In this context, our purpose is to perform a direct simulation of whatever happens to each individual organism in the ecosystem by taking into account all the physically relevant effects, i.e. motion, reproduction and life span. We shall represent the state of the ecosystem by a population of individuals belonging to k different classes. More precisely, two individuals occupy the same class if they belong to the same – preassigned – biomass interval. One should note that the definition of the class is inherent to the rules of the individual behaviour and of the interactions between different classes. These rules are suggested by some real or ideal ecosystems.

In our case, the ecosystem is characterized by the time evolution of the following individual properties: mass, age and spatial location. Our purpose is therefore to perform a time simulation for an ecosystem independently of the more or less well-known sophisticated kinetic models for population dynamics. These models are in general systems of non-linear differential equations whose solutions can be analysed through a computer algorithm (Giró *et al.*, 1985). Nevertheless our aim is rather to obtain a substitute for the real processes, especially in those situations where actual observations are inaccessible because of the system's complexity. These data can then be useful in testing theoretical models, or for the direct control of the system.

Departament Tecnologia Computadors, Fiat. Informàtica, Universitat Politècnica Catalunya, Pau Gargallo 5, 08028 Barcelona, and [1]Departament Termologia, Facultat Fisica, Universitat Barcelona, Diagonal 645, 08028 Barcelona, Spain

**To whom reprint requests should be sent*

Systems and methods

The IBM 3083/XE was used as a main-frame; the operating system of which was VM/SP REL 3. The algorithm was programmed in FORTRAN 77. The computer time and the necessary storage required in order to process the simulation vary according to the nature of the problem and the associated constraints. For instance, if we consider an ecosystem of about 10 000 individuals (as described in the implementation paragraph), we need 500 kbyte of memory and the computation time amounts to about 3 s per time step.

When the run needs a large amount of c.p.u. time, it is divided into different parts and a special storage algorithm for the partial results is needed in this case. The input DATA include all the control parameters. Our algorithm uses the random subroutine of the series of the NAG FORTRAN Library, Mark 11 (cycle length: 2^{57}).

Algorithm

The program – the Barcelonagram – is a simulator of an ecosystem of several classes. We consider first the sets of nutrient particles that we shall call 'nutritons' (Giró *et al.*, 1985), the nourishing substrates for individuals. We also consider the following phenomena with the corresponding characterizations.

Motion: r_m, the radius of the area in which an individual moves at random.

Nutrition: sort of nutrition (other classes, common substrate, etc); Δt_a, the time interval between two consecutive nutrition consumptions; ΔM_{max} and ΔM_{min}, maximum and minimum quantity of mass that individuals can ingest at one time; r_a, the radius of the area in which an individual searches nutritons.

Growth: α, the relation between the consumed mass and the increasing individual biomass (metabolic efficiency); Δt, aging for each times step of the simulation.

Reproduction: set of reproducing conditions (age, mass, etc.); set of characteristics of new individuals (mass, spatial location, etc.); set of characteristics of the ancestor after reproduction (mass, etc.).

Death: t_{max}, age of death; set of factors affecting the age of death (available nutritons, population density, etc.).

Two basic ideas for the simulation of liquids in physics are considered in the Barcelonagram: (i) the periodic boundary conditions and (ii) the cellular structure method. The former enables the simulation of an infinite system by means of a finite number of individuals. Space is supposed to be divided into square cells. The principal cell – the cell under consideration – is in contact with eight identical cells (true copies of the central cell) through completely transparent walls. In other words, when one individual leaves the central cell then the corresponding image enters through the opposite wall. The second idea, the cellular method, is one of the time-honoured tools in molecular dynamics (Giró *et al.*, 1980) for its efficiency (time saving) makes the simulation actually viable. The cellular method consists basically in considering the principal square to be divided into subcells and it is particularly appropriate for the representation of our ecosystem (Figure 1). The location of one individual is indeed guaranteed by determining which subcell is lodging this individual at any time. Figure 2 shows the flow-chart of the simulation program. The modular structure provides for versatility concerning very different situations. We describe now the essential parts of the Barcelonagram.

Data input

The input data determine the general characteristics of the ecosystem: number of classes; occupation of each class (number of individuals); characteristic parameters of each class (mass, life time, area of influence, etc.); size of the principal cell and NSA, the number of subcells to be considered.

Cellular structure (subroutine TRADUC)

The number of subcells NSA corresponding to the principal cell (called A), and the radius of action NC (maximum radius of motion or nutrition) determine the number of subcells NSB of the extended cell (called B), that is to say, the original central cell plus the subcells given by the periodic boundary conditions (Figure 1).

The objective of such a subroutine (Table I) is first the numeration of both cells A (FOR 1 to NSB) and B (FOR 1 to NSB). This arrangement is performed using the spatial coordinates (x,y) of the cells. The second objective is the creation of the vector IAB which determines the anti-image LA (in A) of each subcell LB (in B) [IAB(LB)=LA].

Interaction matrix (subroutine ITESUB)

This subroutine (Table II) assigns to each subcell of A all the subcells of B interacting with A, independently of whether they are images or not (Figure 1). It starts with itself and follows

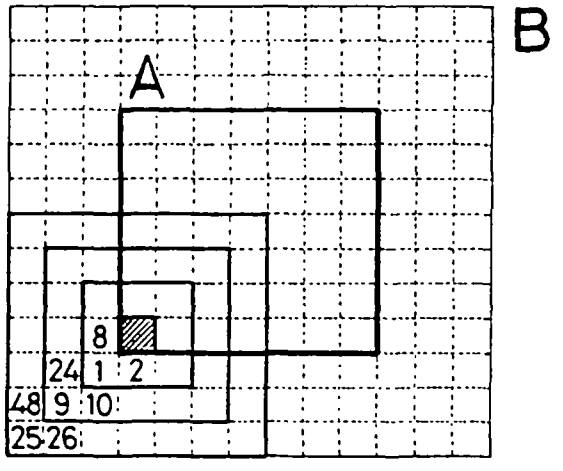

Fig. 1. The cellular structure method assigns to each subcell (dark in the figure) of the principal A all (listed) subcells of the extended cell B (namely, the cell A plus the subcells given by the periodic boundary conditions) interacting with the mentioned shaded subcell. In this case the radius of action NC (the maximum radius of motion or nutrition) corresponds to three layers of subcells.

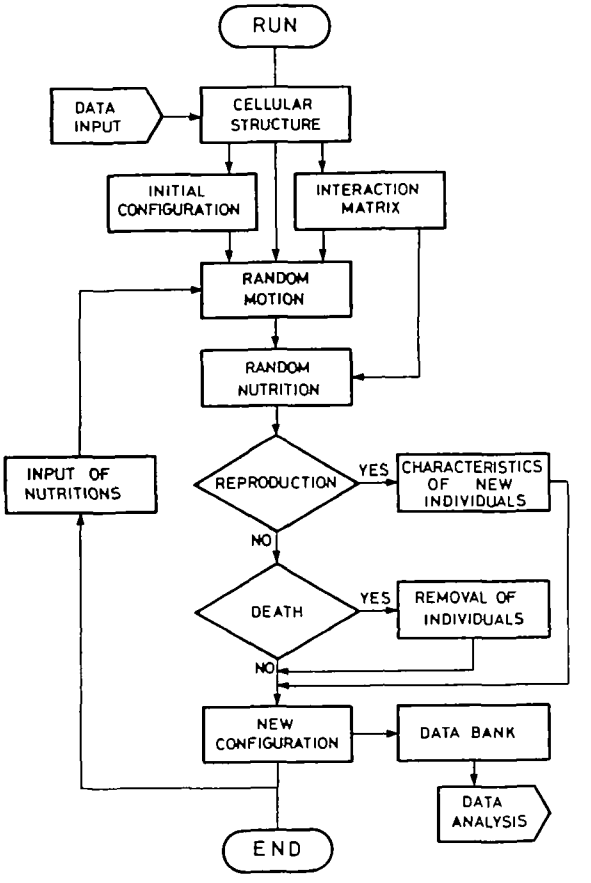

Fig. 2. The flow-chart of the Barcelonagram.

with the successive concentric layers of the surrounding subcells. Once the list is created, the subcells of each interaction layer are rearranged at random. This rearrangement avoids the appearance of privileged directions. The 48 subcells that interact with the first subcell of A are labelled in Figure 1; in this particular case, the maximum radius of action corresponds to three layers of subcells. It should be noted that the area of action can be continuously modified (for the characterization of different classes) by means of a multiplicative factor representing the contribution of each layer of subcells.

Initial configuration

This subroutine creates the initial configuration of the ecosystem. We start with the random distribution of the individuals of each class in the A subcells. We moreover fix at random the individual values of mass and age, taking into account – if it is the case – the part of the young population (without reproduction capacity). The subroutine also establishes the nutritons' distribution in A (Call INPUT NUTRITONS).

Iterative part of the program

Starting from the initial configuration and according to the characteristics of each class, the program generates the time evolution of the ecosystem. In each time step the following processes are therefore considered:

(i) Input of nutritons.
(ii) Age increment of each individual ($=\tau$).
(iii) The identification of individuals whose turn it is to move or to eat.
(iv) Once the motion is performed individuals start to eat at random the available nutritons in the corresponding area of action.
(v) Each individual is tested for the minimum reproduction conditions (age, mass) and, if they are satisfied, the characteristics of the new individual are fixed (age, mass and birth subcell).
(vi) The individual age is checked; if it reaches the maximum value, the individual is removed from the ecosystem. This maximum age can be advanced as a virtual aging due to a lack of the available amount of nutritons.

Table III shows a detailed scheme of this iterative part of the program.

Table I. Procedure TRADUC

```
C ISA Number of subcells per side of the principal square (ISA = 7,
      Figure 1)
C ISB Number of subcells per side of the extended square (ISB = 13,
      Figure 1)
C   Subcells numeration of both systems
C     Numeration of the principal square, A
      K = 0
      FOR J ← 1 UNTIL  ISA  DO
        FOR I ← 1 UNTIL  ISA DO
          K = K +1
          NSA(I,J) = K
        END DO
      END DO
C     Numeration of the extended square, B
      K = 0
      FOR J ← 1 UNTIL  ISB  DO
       FOR I ← 1 UNTIL  ISB DO
         K = K + 1
         NSB(I,J) = K
       END DO
     END DO
C    Correspondence of the subcells of B into the subcells of A
     FOR JJ ← 1 UNTIL  ISB  DO
       FOR II ← 1 UNTIL  ISB DO
         We look for the coordinates (I,J) of the subcell of A being the
         image of any subcell of B with coordinates (II,JJ)
         JX(1) = II
         JX(2) = JJ
         FOR L ← 1 UNTIL 2  DO
           KX = – NC
           IF JX(L) ≤ NC THEN KX = –NC + ISA
           IF JX(L) > NC+ISA THEN KX = –NC – ISA
           JX(L) = JX(L) + KX
         END DO
         LA = NSA (JX(1), JX(2))
         LB = NSB (II,JJ)
         IAB(LB) = LA
       END DO
     END DO
     RETURN
     END
```

Table II. Procedure ITESUB

```
C NG maximum number of layers
C NS number of subcells in A
     FOR L ← 1 UNTIL  NS  DO
           We search the coordinates (I,J) of the subcell L
           IA = I – NG
           IB = I + NG
           JA = J – NG
           JB = J + NG
            FOR II ← IA UNTIL  IB  DO
                 FOR JJ ← JA UNTIL  JB  DO
                     We search the anti-image LA of the subcell
                     LB= NSB (II,JJ) (Call TRADUC)
                     We look for the interaction layer NN
                     containing LB (1 ≤ NN ≤ NG)
                     We notice that subcell LA belongs to the layer
                     NN, and its interaction with L
                 END DO
            END DO
           Disarrrangement at random of subcell belonging to the
           same layer NN (Call RANDOM)
     END DO
     RETURN
     END
```

Table III. Iterative part of the program

```
C NJ Number of individuals of the class J (J = 1,2, . . . . . n)
C n  Number of classes
     FOR J ← 1 UNTIL  n  DO
          FOR I ← 1 UNTIL  NJ  DO
           Aging   Age = Age +
                If Nutrition THEN list
                   WHILE list ≠ 0 DO
                     Random selection of one individual (from
                     the list) that starts nutrition (Call
                     RANDOM)
                     Starting of nutrition by random motion into
                     its spatial area of influence (Call
                     RANDOM)
                     Identification of the destination cell (Call
                     CELLULAR STRUCTURE)
                     Random searching of nutritons into the
                     spatial area of influence (Call
                     INTERACTION MATRIX)
                     Increasing of mass accordingly to
                     metabolism
                     IF it reaches the value of the reproduction
                     biomass THEN
                       Birth of a new individual:
                         Modification of the ancestor's value of
                         mass
                         Determination of the parameters of the
                         new individual (location, mass, age,
                         etc.)
                       ELSE ← IF it reaches the maximum age
                       or further conditions *THEN Death (it is
                       written off)
                     END-IF
                   END-WHILE
                END-IF
          END
     END
```

[a]If the individual doesn't obtain a sufficient amount of nutritons during a prefixed number of time-steps. See Figure 4.

Implementation

We next discuss the preliminary results of the Barcelonagram in some simple situations. Our first purpose is the time evolution of the biomass production in ecosystems exhibiting the following properties:

(i) All individuals pertain to a single class.
(ii) There is one single class of common substrate (nutritons)
(iii) $r_m = r_a$.
(iv) The area of action corresponds to the very central subcell and to the first layer of surrounding subcells.
(v) $\Delta t_m = \Delta t_a$.
(vi) Reproduction occurs at a certain individual mass value, M_{max}.
(vii) The ancestor individual changes its mass according to: $M_N = M_{max} - M_i$ where M_i is the mass of the new individual.
(viii) No direct interactions are considered between individuals.

This strongly restrictive condition nevertheless respresents a high number of real natural or artificial situations, i.e populations of fishes [groups of a high number of individuals ($\sim 10^4$) having plankton – or some special prepared food – as a unique nourishing source], bacterial cultures, etc. Some different environmental constraints can be easily imposed on such systems, namely, a constant total biomass (individuals plus nutritons), an isolated boundary enclosing a certain initial quantity of nutritons, a constant input of nutritons, etc. The preliminary results match satisfactorily with global deterministic models and provide some specific insight concerning the domain of reliability of such theoretical models.

In an earlier paper (Giró *et al.*, 1985), we reported an investigation of dynamic laws of population versus the data of computer simulation. The former were represented by the

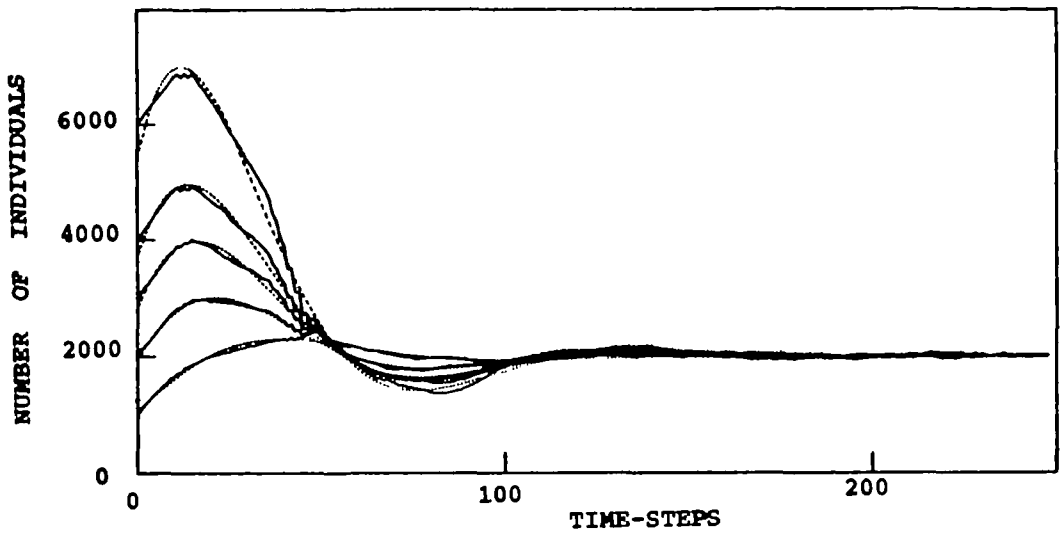

Fig. 3. Time evolution of individuals belonging to the same class and starting with different initial populations. The continuous lines represent the Monte Carlo computer simulation. The dashed lines are the fitted analytical solutions of the differential equations (1).

differential equations

$$\begin{aligned} n &= -k_1 n + k_2 s \\ s &= -k_3 n + k_4 \end{aligned} \quad (1)$$

where n is the number of individuals, s the number of nutritons and k_1, k_2, k_3 and k_4 positive constants. The population adapts itself to the external constraints, i.e. $n(\infty) = k_4/k_3$ following the typical transitory evolution of a damped oscillator subjected to an external force. The solutions recall, if $n(0) < n(\infty)$, the logistic sigma-like curve to the final state $n(\infty)$ and the overdamped situation shows, in particular, the same qualitative behaviour predicted by the Lotka–Volterra equations for the parasite–host population cycles in which a cross-term kns is included (Svirezhev and Logofet, 1983).

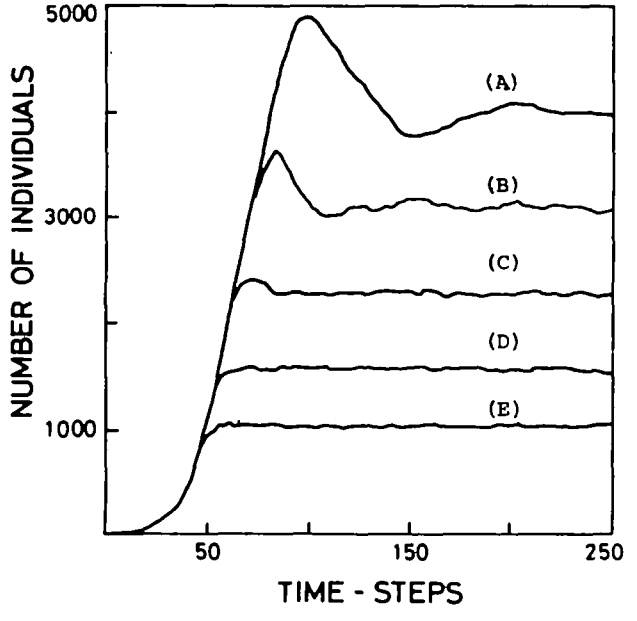

Fig. 4. The shifting (from A to E) of the growth curve from the former case (Figure 3) towards the sigma-like logistic curve for increasing limitating nutrition conditions, namely, the maximum time interval (NA) that an individual may keep itself alive without nourishing. The curves correspond to the following values: NA(A)= ∞; NA(B)= 16; NA(C)= 8; NA(D)= 4; NA(E)= 2.

In ecology, as in other sciences, it is important to distinguish between equations or 'laws', whose justification is that they describe the observed or simulated relations between two or more variables, and those which have in addition some 'microscopic' justification in terms of the known or postulated behaviour of the components of the system. This is the aim of both the alternative equations (1) and the computer simulation. The matching between the detailed and the overall treatments is successfully explored by the program minimizing a goodness-of-fit criterion. The preliminary results are indeed encouraging. First, the Barcelonagram provides, as predicted by the mathematical theory, an approach to the imposed stationary state, independently of the initial state of the system (Figure 3). This behaviour may be an aperiodic damping (a typical sigma-like curve) or a damped oscillator, according to the specific properties of the different classes. A consistency check is easily performed by observing the effect of the shifting of one behaviour to the other in both descriptions if one changes accordingly the internal laws in the Barcelonagram or the appropriate constants in the deterministic equations (Giró *et al*, 1985). Moreover, the well-known shapes of the experimental growth curves can be obtained by the simulator introducing the realistic effect of the limitating nutrition resources. Figure 4 exhibits the tendency to such a sigma-like curve by increasing the 'penalization' due to the lack of available nutritions (see footnote of Table III).

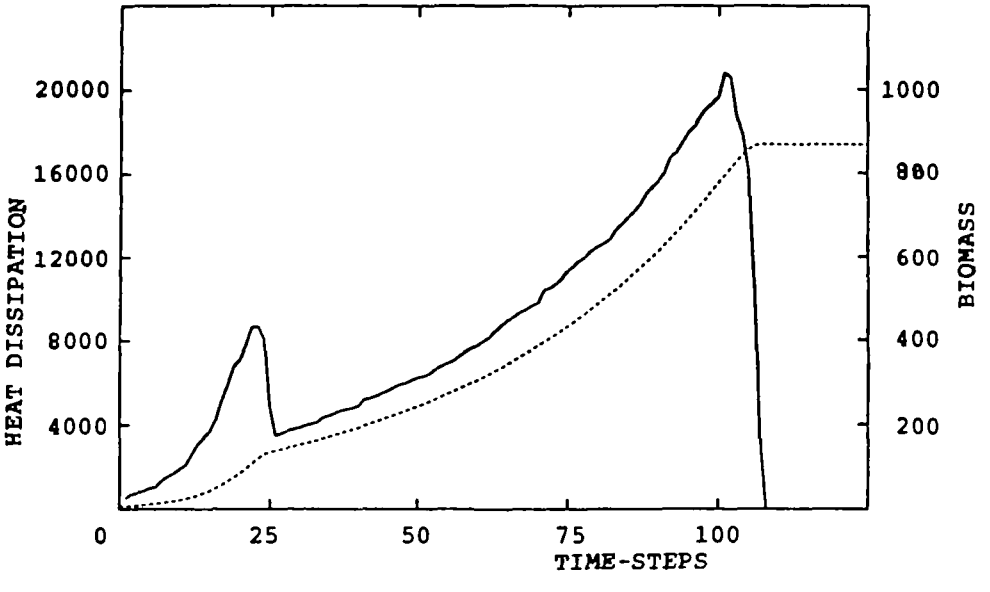

Fig. 5. Time evolution of heat dissipation (solid line) and biomass (dashed line) in arbitrary units obtained with the Barcelonagram. The behaviour is strongly close to that observed by microcalorimetry in similar environmental conditions for the *Serratia marinorubra* strain IP75 (Bermúdez and Wagensberg, 1985).

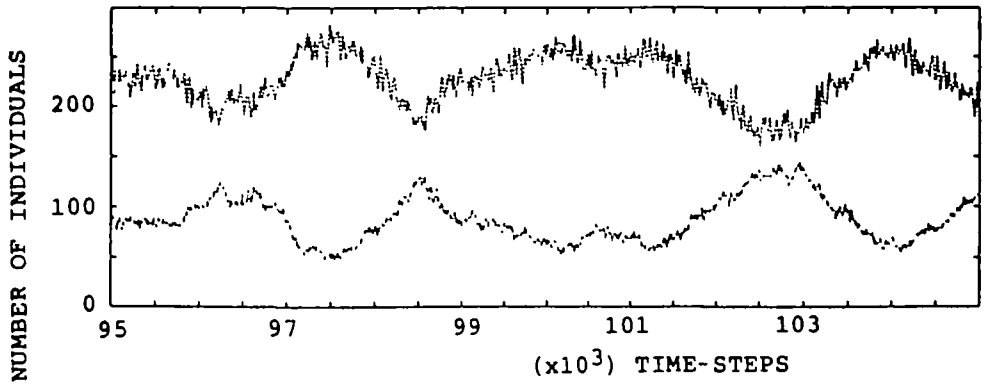

Fig. 6. Time evolution of the population in a two-class ecosystem obtained with the Barcelonagram. The system has been proved to be stable until 2×10^5 time-steps.

Discussion

Our simulation provides a useful connection in order to identify the constants appearing in the deterministic models in terms of detailed random behaviour. This is, we believe, of great interest for the management of biomass production plants where the time simulation of the type presented here is a substitute for inaccessible observations. This technique is therefore more justified for systems of increasing complexity. On the other hand, it provides a tool to determine the limits where the theoretical approaches break down, i.e. the domain of reliability of analytically idealized equations (Giró *et al.*, 1985). We have indeed discovered some circumstances, usually ignored in such models, becoming relevant (time delays, random events, non-linearities, memory effects, statistical meaning of macrovariables, etc.).

The Monte Carlo simulation is also a tool to be considered for further generalization and it is in these more complex systems where the method would readily find a relevant application. The stability of ecosystems can be sought, for example, in many interacting species systems for a wide range of energetic conditions such as space-time dependent surrounding constraints. In particular, Figure 5 shows the starting point of a promising perspective: the simulation of the bacterial growth together with the corresponding heat dissipation curve. Our preliminary (qualitative) results in this case suggest the possibility of an important bridge between microcalorimetry (Bermúdez and Wagensberg, 1985) and the investigation of microbiological metabolism. Further quantitative results for the particular strain *Serratia marinorubra* IP75 growing in complex media are to be reported soon. Up to now we have realized with the Barcelonagram the critical nature of the value range of parameters which allows the stabilization of the two classes competing for a constant input of nutritons, as can be seen in Figure 6. Another relevant point concerns the biomass distribution of individuals at the stationary state predicted by some informatic–thermodynamic models (Lurié and Wagensberg, 1983, 1985).

To sum up, the Monte Carlo simulation plays the role of the experimental observations with perhaps the same handicap as in molecular dynamics, that is to say, less credibility concerning what is actually happening in nature; but it has nevertheless the same relevant list of advantages. Simulations do advantageously replace experiments in real complex systems, for, in the latter, the control of the external constraints can be very difficult, the direct observations themselves are almost impossible to record reliably, and the necessary experimental tests in man-made ecosystems are not, in principle, economic or comfortable. The simulation is, moreover, specially interesting to apply in the neighbourhood of critical situations in order to test the sensibility of a many-species ecosystem in the face of internal or environmental fluctuations, a central problem regarding the concepts of biological adaptation versus internal or external noises.

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