Some speculation on simulation

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Systems and models

For more than 30 years, considerable attention has been paid in the engineering sciences to the analysis of complex, dynamic systems and with considerable success. The approach, which is now being adopted in the biological sciences, is characterized by the terms: systems, models and simulation. A system is a part of reality that contains interrelated elements, a model is a simplified representation of a system and simulation may be defined as the art of building mathematical models and the study of their properties in reference to those of the system.

Although any model should have definite goals, be lucid and achieve its objective, it seems in practice that goals are too often described in such broad terms that sufficient lucidity is reached only for the initiated and that the models are achieving less than expected by the biologists. For these reasons the word 'art' rather than 'science' is used in the definition of simulation.

It follows from the definition that a model is a system, but the reverse may be true as well. A work of art is a simplified representation or a model of the vision of the artist. A machine is a model of the conception of the engineer and it performs certainly worse than anticipated. And when an engineer applies simulation, he develops models that are in between his conception and reality. The ultimate machine is in fact a model of his simulation model, that is a simplified representation of his mental conception.

Although some would like it otherwise, biological systems are not simplified representations of the conception of the biologist and the inversion of the terms, models and systems does not make any sense. Therefore, it may be that the approach that has been so successful in engineering is not as useful in biology. Fools rush in where wise men fear to tread, and much of the rushing in this field of simulation in biology is done by agronomists, perhaps because they are fools, but may be because they are concerned with systems in which the technical aspects overrule the biological aspects.

State-variable approach

A file with data on an ecosystem may be called a model, but then a model without purpose and lucidity. Uses of the data may be formulated and then lucidity may be introduced by a treatment of the data. This may result in maps that represent aspects of the ecosystem, or in statistical analyses which summarize some of the interrelations. Dynamic models are obtained if the time dimension is introduced during the collection and treatment of the data. But the models remain descriptive, showing only the existence of relations between elements, without any explanation, which is, of course, not their purpose to begin with.

However, models that have the purpose of explaining systems are possible in biology, because various levels of organization are distinguished in this science, as in any other natural science. These different levels of organization may be classified, according to the size of the system and time constants involved, as those of molecules, cell structures, cells, tissues, organs, individuals, populations and ecosystems. Models that are made with the objective of explaining are bridges between levels of organization, which allow the understanding of larger systems with the larger time constants on the basis of the knowledge gained by experimentation on smaller systems with smaller time constants. In this way the properties of membranes may be understood better by studying molecules and the properties of ecosystems by studying species.

For models that claim to be of the explanatory type, the state-variable approach is gaining wide acceptance. These models are based on the assumption that the state of each system at any moment may be quantitatively characterized and that changes in the state may be described by mathematical equations. This leads to models in which state, rate, and driving variables are distinguished.

State variables are quantities like biomass, animal number for a species, the amount of nitrogen in soil, plant or animal, the water content of the soil; roughly those variables that can still be measured when time stands still as in the world of the Sleeping Beauty are state variables.

Driving variables characterize the interactions at the boundaries of the system and are continuously measured. Examples are macrometeorological variables like rain, wind, temperature and radiation, and the food supply or migration of animals over the boundaries of the system. It depends on these boundaries, whether the same variables are driving, state, or rate variables. For instance, the heat stored within a vegetation canopy is a state variable when the system includes micrometeorolocal aspects, but a driving variable which has to be measured when the micrometeorological aspects are excluded from the system.

Each state variable is associated with rate variables that characterize their rate of change at a certain instant as a result of specific processes. These variables give the values of flows of material between state variables, for example, between vegetative biomass and grazing animal. Their value depends on the state and driving variables according to rules that are based on knowledge of the physical, chemical and biological processes that take place and not on a statistical analysis of the behaviour of the system which is being studied. This is the most important distinction between models that describe and models that attempt to explain.

New values of the state variables are found after calculating all rates; the computing process is usually repeated at given time intervals. In its most elementary form this is a process of numerical integration and the simulation program may be replaced by an analytical solution in cases where the equations are simple enough, but this is a rare occurrence.

Most models are too complicated and contain too many discontinuities and random processes to allow straightforward application of numerical integration methods. Various simulation techniques with different 'world views' have been developed to handle such models. Those originating from operation research studies are event-oriented. It is assumed that in general nothing changes and, on the basis of the state of the system and the assumed random processes, the time of occurrence of the next rare event is computed. Time is advanced then towards this moment and the event is executed. The simulation techniques that originated from the engineering sciences assume that continuous changes are dominant and incorporate standard numerical integration techniques. Both simulation techniques are continuously incorporating elements of the other, a process that has advanced to such an extent that the one-time unavoidable discussion on the superiority of the approaches is dying away. At present much more attention is paid to iterative use of computers.

Especially for the uninitiated, attempts are made to simplify simulation programs into relational diagrams, often according to a method that was developed by Forrester (1971) to represent models of industrial systems. An example of such a relational diagram is in the contribution of Jameson. The state variables are given within rectangles (□) and the flow of material (water, carbon, nutrients) by solid arrows. The rate control of these flows is presented by the valve symbol (▷◁). The driving and decision variables are given within hexagonals (⬡). The dotted lines indicate which state or driving variables affect which rate, without indicating the quantitative aspect: these are the flows of information that are considered.

Rates are not dependent on each other in these state determined systems. Each rate depends at each moment on state and forcing variables only and is therefore computed independently of any other rate. Hence it is never necessary to solve n equations with n unknowns. An example may be needed. It is clear that the rate of growth of a plant, as measured by the increase in weight of its structural tissues, is closely related to the rate of photosynthesis of the leaves. In a state-variable model, this dependency is a result of the simultaneous operation of two independent processes. Photosynthesis contributes to the amount of reserves and this amount is one of the states that determine the rate of growth. At the onset of darkness, photosynthesis stops immediately, but growth proceeds until the reserves are depleted or even longer but then at the expense of existing tissue.

Some practical problems

The number of state variables that may be distinguished in an ecosystem are depressingly large. They concern not only primary producers, consumers and decomposers, but also the various species, their number, size, age, sex, stage of development etc. For plants, not only the weight and surface area of the leaves are of importance but also their nitrogen and mineral content, their enzymes and other biochemical characteristics. One can continue in this way and therefore a model that is based on full knowledge of all biological, physical and chemical phenomena that occur is never realised. Models are simplified representations of systems and the simplification manifests itself by the limited number of state variables that are considered.

In analogy with other approaches, it is assumed that considerable reduction of the number of state variables may be obtained by limiting the boundaries of the model and to focus the interest on those aspects where interest or understanding is most wanted. Then processes can be ordered with respect to their importance and only processes within the limited focus need be handled in detail.

It may be desirable, to focus attention on certain aspects, to have greater detail in those aspects and less detail in others. A modular approach to construction of the model is more manageable than constructing a single large model, i.e. the system can be split into sub-systems or modules like soil water, plant growth, nitrogen cycling, animal food consumption, and growth, etc. Likewise greater lucidity may be obtained by adapting the hierarchial approach discussed by Goodall in this book whereby different levels of resolution and different time-steps can be developed for different aspects of a sub-system or module. For example plant growth might be simulated on a daily time-step from photosynthesis and respiration of individual leaves on an hourly time-step.

The number of state variables that can be considered in any model is very limited, not so much because of the size of the computer or the cost of computer time, but because the research effort that can be invested in any one problem is limited. Models that contain about a hundred state variables are for this reason already very large, but at the same time they may be small compared with the complexity of the ecosystems that are considered.

For each purpose there is somewhere an optimum in the number of state variables that should be considered. At first the applicability of the model to the real world problem increases with increasing number of state variables, but then it decreases again because the addition of new state variables diverts attention from state variables introduced earlier because they were considered more important. The heuristic process of obtaining a set of state variables in order of their importance takes much time and many modelling efforts in ecology are sometimes explicitly but mostly implicitly geared towards this goal.

The validity of a dynamic model is thus always open to question but Wigan (1972) suggested that the following methodology is useful in minimising internal errors and maximising the validity of a model. He proposed five stages. 1) *Postulates* – the selection of basic assumptions of form and interaction on which the remaining stages are based. 2) *Fitting* – having selected a set of parameterized functions based on the postulates, fit 'best' values to these functions according to defined criteria of 'best' fit. 3) *Calibration* – given a set of fitted functions (or sub-models), calibrate their interrelationships with direct reference to the overall behaviour of the model and the data which the model aims to reproduce (sensitivity analyses). 4) *Identification* – ensure that the detail of the calibrated model is justified by the available data (and find the best reduced form if required). 5) *Validation* – the process of discriminating between different sets of postulates by reference to fresh data not used in the setting up, fitting and calibration process. These principles, written by an engineer concerned with modelling a transportation system apply equally to ecosystems. If such rigour was applied by biologists more often perhaps the value of their models would be greater.

In this way simulation may aid the understanding of important aspects of complex systems, in such a way that their behaviour is visualized and a guide to their management is obtained. But solutions are only accepted as such, if methods to falsify them are available, or to state it more positively, if they can be verified or their usefulness can be proven. Are there models that can be validated? Yes, but only of systems that are repeatable or recur. Only then may the model be derived from the analyses of some systems and validated on others. Examples of repeatable systems are microbiological (manufacture of vinegar), agricultural (growth of maize) or industrial (manufacture of cars). Examples of recurring systems are stars, individuals of a species and ecological systems with so much resilience that after disturbance the original course of development is restored in due course (peat bogs). These recurring ecological systems appear to the observer at different places at the same time but in different stages. The strength of the field-ecologist lies in his ability to interpret as a time series in one place what is observed in different places at one moment. Repeatable systems can always be analysed by experimentation, but recurring systems sometimes only by observation. There is at present a strong emphasis on the experimental analysis of recurring ecological systems and this is justified because disturbances are dampened and destruction of the system during experimentation may be acceptable because there are many of them.

But there are also unique ecological systems or ecological systems with unique aspects. These are systems in which development is not governed by negative feedback, so that their development is diverse, although the origin may be the same. Other systems are unique because of the geographical situation, like some estuaries, lakes, islands and of course the world as a whole. Models of unique systems are concepts that cannot be validated experimentally but only more or less verified by observation of the behaviour of the real system over time. They remain therefore speculative models. The faith in speculative models is strengthened if similar methods of systems analysis applied to repeatable or recurring systems lead to validated models that cannot be falsified. Such models exist of physical systems: speculative models that predict the chances of flooding on the basis of an analysis of the physical processes are trusted although sufficient floods for verification never occur within a human lifespan. Whatever the model predicts, the dykes are strengthened as soon as one flood takes place and this proves that trust of this kind has its limits. Speculative models of ecological systems cannot be trusted as yet, because few models that are properly validated exist and the principles of model-building in ecology are still being developed. This certainly holds for so-called 'world models' unless their results are so obvious that the proper conclusions may be drawn without sophisticated techniques.

But if a speculative model of a unique system is sufficiently trusted, can it be used? For this purpose it is at least necessary to initialize the model so that the values of all the state variables have to be determined within such a short time span that they do not change materially. And this should be done without disturbing the unique system to such an extent that its course of development is affected.

In the final analysis it may appear that the ecologist is in the same position as the outmoded physicist, who claims that it is only necessary to determine at the same time the position, mass and velocity of all gas atoms in his room to predict their future. He may be in an even worse position because he has to live with or even within his unique system and cannot escape the problem by using the law of averages.

References

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