



Jun 25th, 2:00 PM - 3:20 PM

## Models and modeling in the environmental sciences: Between epistemology and practice

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Gualtieri, Carlo; Mihailović, Dragutin T. Prof.; Kapor, Darko Prof.; Crvenković, Siniša Prof.; and Arsenić, Ilija Dr., "Models and modeling in the environmental sciences: Between epistemology and practice" (2018). *International Congress on Environmental Modelling and Software*. 17.  
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# MODELS AND MODELING IN THE ENVIRONMENTAL SCIENCES: BETWEEN EPISTEMOLOGY AND PRACTICE

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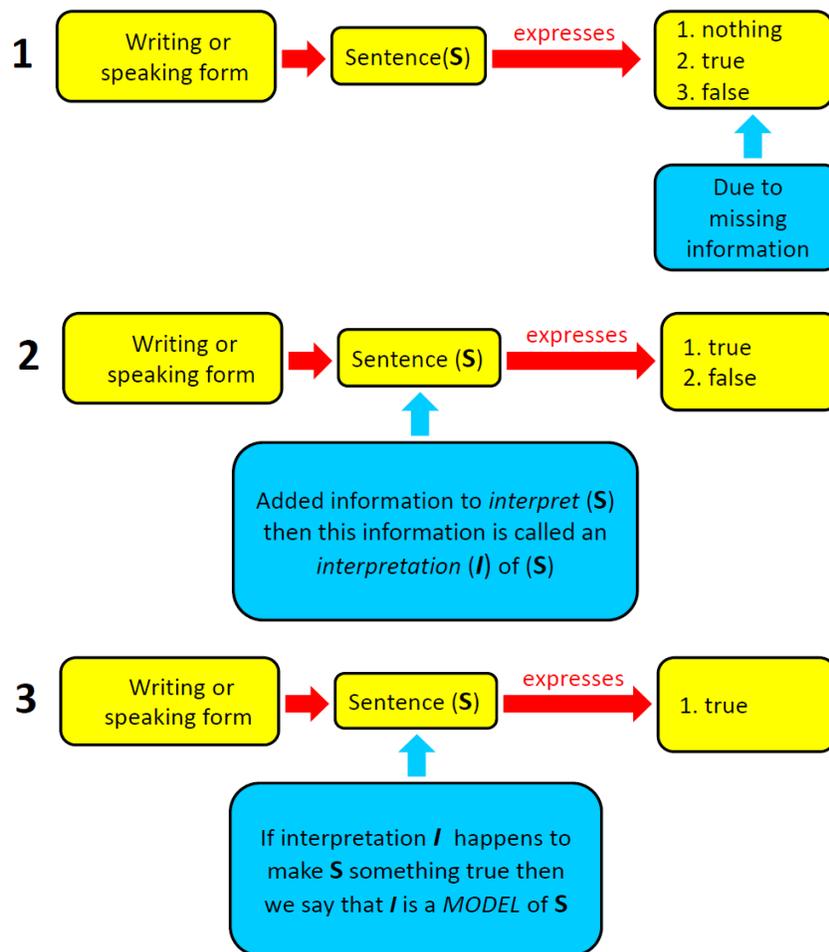
**Abstract:** Designing the models and their use in computer simulation in the environmental sciences inherently involves many epistemological questions. Although practical considerations often overruled the problems of epistemology sometimes it is necessary to make basic epistemological choices, especially in modeling. In sciences and accordingly in environmental ones for many reasons modelers ignore non-linearity of phenomena and processes. If we decide to linearize “the object of modeling” then we use linear equations where the variables and their derivatives must always appear as a simple first power. The theory for solving linear equations is rather well developed one because linear equations are simple enough to be solvable. The shortcoming of this approach is that it neglects that many aspects and phenomena, even important ones, which remain hidden. However, if we decide to follow as much as possible the existing nonlinearities in the object that we model we have to consider the following key points: (i) Model choice; (ii) continuous-time versus discrete-time in building the model and (iii) model predictability (Lyapunov time). Our considerations will be supported by some examples in the modeling of environmental processes.

**Keywords:** Model Theory, generalized logistic map, heuristic models, continuous-time versus discrete-time in building the model, model choice, model predictability (Lyapunov time)

## 1. INTRODUCTION

The human mind (encapsulating the human intellectual sphere) deals with various intellectual activities such as philosophy, mathematics, the sciences, art, as well as experiences that fall outside of the deliberate, such as unconsciously assimilated experiences falling under the category of intuition (Damasio, 1994). Since the authors of this study are not fully familiarized with expressions belonging to the domain of psychology and related disciplines, already at the beginning of the study we will make a distinction between words “intellectual” and “mind”. “Intellectual” is a synonym of “mind”. As nouns the difference between intellectual and mind is that intellectual is an intelligent, learned person, especially one who discourses about matters while mind is the ability for rational thought. As an adjective intellectual is belonging to mental process (mental function), which is all the things that individuals can do with their minds. These include perception, memory, thinking (such as ideation, imagination, belief, reasoning, etc.), volition, and emotion (some authors argue about term emotion; thus Solomon (1976) claims that emotions are actually just assessment, so in that sense they can fall under the concept of cognitive). Sometimes the

term cognitive function is used instead. In this study these words will be used synonymously, i.e. regardless on word which is used, the reader will understand its meaning from the context of the sentence. In mathematics, Model Theory studies classes of mathematical structures (for example, groups, fields, graphs, and universes of set theory) from the standpoint of mathematical logic. The objects of study are models of theories in a formal language. In other words Model Theory is the part of mathematics showing how to apply logic to the study of structures in pure mathematics reaching the high point of abstraction; on the other, it has instantaneous applications to every-day mathematics. As noted by Chang and Keisler: „Model theory is the branch of mathematical logic which deals with the connections between a formal language and its interpretations, or models.” (Chang and Keisler, 1990). The intrinsic dogma of Model Theory is that mathematical truth, like all truth, is relative. Namely, a statement may be true or false, in dependance on how and where it is interpreted, as we tried to show schematically in Fig. 1.



**Figure 1.** Flow diagram of the model definition.

This is not necessarily due to mathematics itself, but is a consequence of the language that we use to express mathematical ideas. When we want to model a phenomenon we have to build a formal theory that describes and explains it. In other words, we model a system or structure that we plan to build, by writing

a description of it. These are very different senses of *model* from that in model theory: the model of the phenomenon or the system is not a structure but a theory, often in a formal language. One of the intellectual efforts are oriented towards creating (designing, making, constructing, etc.) the models. The word “*model*” is highly ambivalent, thus there is no uniform terminology used by either scientists or philosophers. Designing the models and their use in computer simulation in the environmental sciences inherently involves many epistemological questions. Although practical considerations often overruled the problems of epistemology, sometimes it is necessary to make basic epistemological choices, especially in modeling. Except the introductory comments, in this study we will not deal with the epistemological problems associated with models and modeling. Hence, the second part of the title should not be understood as a hyperbolization of the story that will follow, but only as an indication of the need and importance of raising the design of the model in the science to an even higher level. Here, a model is considered to be a representation of some object, behavior, or system that one wants to understand. In this study we realize our message through the following key points of model building: (i) Model choice; (ii) continuous-time versus discrete-time in building the model and (iii) model predictability (Lyapunov time).

## 2. MODEL CHOICE

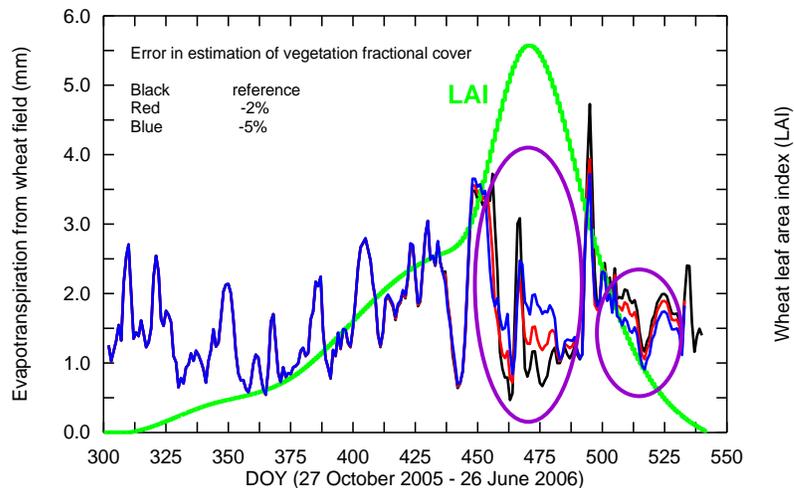
In choosing the model scientists often apply a *heuristic* technique that could be defined as any approach to problem solving that makes use of a practical method not guaranteed to be optimal or perfect (this word is used metaphorically), but sufficient either for the immediate goals or until the better approach is reached. Where discovery an optimal solution is not possible or impractical, heuristic methods can be used to speed up the process of finding a satisfactory solution. We meet the heuristic technique in many sciences, in particular technical and environmental, when some phenomena cannot be always expressed through time-dependent equations whereas they have to be parameterized. For example, in modeling the turbulence while designing the land surface schemes, modelers encounter with many problems in modeling the turbulence above and inside the canopy. Thus, prevailing problems due to the representation of turbulence inside the canopy are in a plastic manner described by Sellers (1987).

He said: “*We have mentioned before that use of “K-theory” within the canopy may be physically unrealistic, but because it yields reasonable results we shall use this method until suitable second-order closure can be applied to the problem*”. Interestingly, depending on modelers’ requirements, this model can be supplied (for example, land surface schemes) with parameters, which are either less (in atmospheric models) or more (in crop micrometeorology simulations) precisely selected. In both case the model can give satisfactory results.

We illustrate this situation with an example of the calculation of the evapotranspiration in the LAPS surface scheme (Mihailovic et al., 2010) as it is visualized in Figure 2.



(c)



**Figure 2.** Variations of evapotranspiration (mm) over the wheat field in Avignon (France) in dependence on error introduced in estimation of the vegetation fractional cover during the growing season (27 October 2005 – 26 June 2006). DOY is the acronym for Day of Year. Simulations were performed by the LAPS land surface scheme (Mihailovic et al., 2010). The pink ellipses round the regions with the highest differences between simulations of evapotranspiration.

The Figure 2a represents typical simulation in crop micrometeorology (where the wheat leaf is seen from the “bug perspective”, i.e., with more morphological and physiological details). The LAPS scheme was run as a stand-alone one for the whole growing season of the wheat. The LAI index was measured every day and then the fractional vegetation cover was estimated via the empirical formula (Boulet et al., 2012). In Figure 2c the time evolution of the LAI is shown by green color while evapotranspiration is depicted by the black one. Then we artificially introduced errors in the LAI values and calculating evapotranspiration. From Figure 2c there are seen the regions (marked by the pink ellipses) with the highest differences between simulations of evapotranspiration. Those differences are huge for the crop micrometeorology simulations. However, looking from the “bird’s eye view” (Figure 2b), i.e., when the land surface scheme is coupled for some atmospheric (general circulation, regional, numerical weather prediction) models (Sellers et al., 1986) with coarser grid-cell, it does not always have to be a problem. At the end, we could say that a “wrong” model can provide good results. The uncertainty or error associated with mathematical modeling has two components: type (1) error, which results from the use of a wrong model with correct input parameters; this uncertainty could result from the selection of a model inappropriate to the phenomena or from a wrong formulation of the model; type (2) uncertainty, which assumes, on the contrary, the use of a correct model with input parameters which are known with some uncertainties; in fact, for example, in water quality modeling, the correct use of a model requires a good characterization of the water body. Therefore, the modeler must define some input parameters, such as kinetic constants, initial conditions, boundary conditions and so on; usually, these parameters are obtained from field study, which are affected by unavoidable uncertainties, or are estimated through empirical expressions which are often inaccurate (Beck, 1987; Oreskes et al., 1994).

How to continue with designing these models in the future? Nowadays, it seems that they are getting better and more helpful. However, because of (i) the nonlinearity of many natural processes, (ii) use of discrete time in solving partial differential equations and (iii) increasing the model complexity [Complexity is that property of a model which makes it difficult to formulate its overall behaviour in a given language, even when given reasonably complete information about its „atomic“ components and their inter-relations

(Kauffman, 1995; Grassberger, 2012)] etc., it seems that these obstacles cannot be bridged in the near future.

Let us add some comments about problems, which we encounter when designing a model. Namely, for some phenomena, described by equation(s), we already know the corresponding laws that can be deduced from symmetry conditions. However, in many other cases, we must determine equations from the general theoretical ideas and experimental data (Kreinovich, 1976). Therefore, we can ask ourselves whether we guarantee that these equations are correct. If the answer is positive then how? Even that we “know” equation(s), but we still are not sure about the values of *parameters* of these equations. Since there often exist many generalizations we derived or designed them for a very wide interval. In particular, there is always present the question when (and how) we can guarantee that these are the right equations, with correct values of parameters. Kolmogorov was among the first who started, in 1960s to analyze this issue. He pointed out two main reasons why a mathematically correct solution to the corresponding system of differential or difference equation cannot be physically possible: (i) there is difference in understanding the term “*random*” in mathematics and physics (also in environmental sciences) and (ii) solutions of the corresponding systems of differential equations which lead to some numbers may be mathematically correct, but they are physically meaningless (Kolmogorov, 1968).

### 3. CONTINUOUS-TIME VERSUS DISCRETE-TIME IN BUILDING THE MODEL

Traditional mathematical analysis of environmental systems tacitly assumes that integers and all real numbers, no matter how large or small, are physically possible and all mathematically possible trajectories are physically possible (Kreinovich and Kunin, 2003). Traditionally, this approach has worked well in physics and in engineering but it does not lead to a very good understanding of chaotic systems, which, as is now known, are extremely important in the study of real world-phenomena ranging from weather to biological systems. Here we consider some issues in modeling pathways in physics, biology and chemistry, i.e. environmental sciences in their broadest context (in short, environmental sciences). They are (a) how to replace given differential equations by appropriate difference equations in modelling of phenomena in environmental world (Van der Vaart, 1973; Gualtieri and Mihailović, 2014) and (b) phenomenon of chaos in autonomous dynamical systems, in particular in solving the energy balance equation for calculation of the environmental temperature.

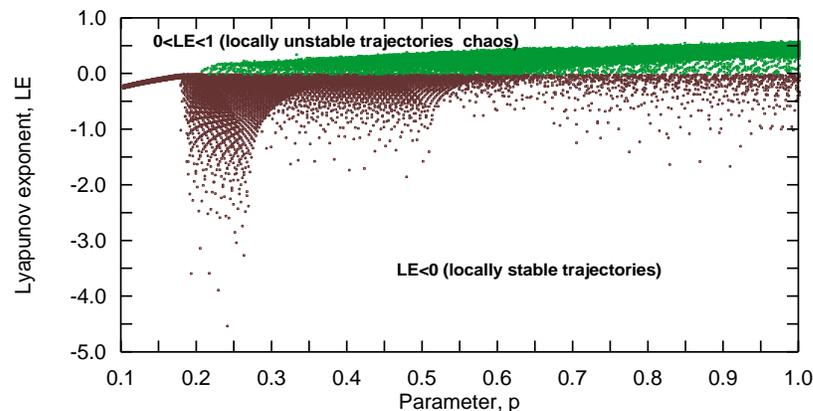
According to Van der Vaart (1973) many models for environmental problems have been and will be built in the form of differential equations or systems of such equations. With the advent of computers one has been able to find (approximate) solutions for equations that used to be intractable. Many of the mathematical techniques have been applied in this area to replace given differential equations by appropriate difference equations. So a huge effort has been invested into the choice of appropriate difference equations whose solutions are “*good*” approximations to the solutions of the given differential equations. This question includes a requirement for better understanding of the fundamental problem: interrelations between classical continuum mathematics and reality in environmental sciences. For many environmental phenomena the “*continuum*” type of thinking, that is at the basis of any differential equation, is not natural to the phenomenon, but rather constitutes an approximation to a basically discrete situation: in much work of this type the “*infinitesimal step lengths*” handled in the reasoning which has lead us to the differential equation, are not really thought of as infinitesimally small, but as finite; yet, in the last stage of such reasoning, where the differential equation rises from the differentials, these “*infinitesimal*” step lengths tend to zero limit: that is where above-mentioned approximation comes in. “*Under this kind of circumstances, it seems more natural to build the model as a discrete difference equation from the start, without going through the painful, doubly approximative process of first, during the modeling stage, finding*

a differential equation to approximate a basically discrete situation, and then, for numerical computing purposes, approximating that differential equation by a difference scheme” (Van der Vaart, 1973).

Let us consider now a typical example of an environmental interface in the nature, where all three mechanisms of energy transfer exist; incoming and outgoing radiation, convection of heat and moisture into the atmosphere and conduction of heat into deeper soil layers of ground. This partial differential equation can be easily solved numerically by stepping either forward or backward in time from known initial condition after it is written in the form of a difference equation. Under some conditions and expected conditions in atmosphere, the energy balance equation can be written in the form of the logistic equation (Mihailović and Mimić, 2012), where variable  $x$  denotes dimensionless environmental interface temperature. Later Mihailović et al. (2016) generalized that equation in the form

$$x_{n+1} = rx_n^p(1 - x_n^p), \quad (1)$$

where,  $x$  is the dimensionless concentration of some biochemical substance within a cell,  $r$  is a logistic parameter,  $0.0 < r \leq 4.0$  and  $p \in (0,1)$  is an intrinsic property of the system dynamics. Thus, by introducing this parameter Mihailović et al. (2016) formalized an intrinsic property of the cell that includes (i) the affinity of genetic regulators towards arriving signals, which determine the intensity of the cellular response and (ii) the affinity for the uptake of signaling molecules. In the same book this equation considered in the context of synchronization and stability of the horizontal energy exchange between environmental interfaces in climate models.



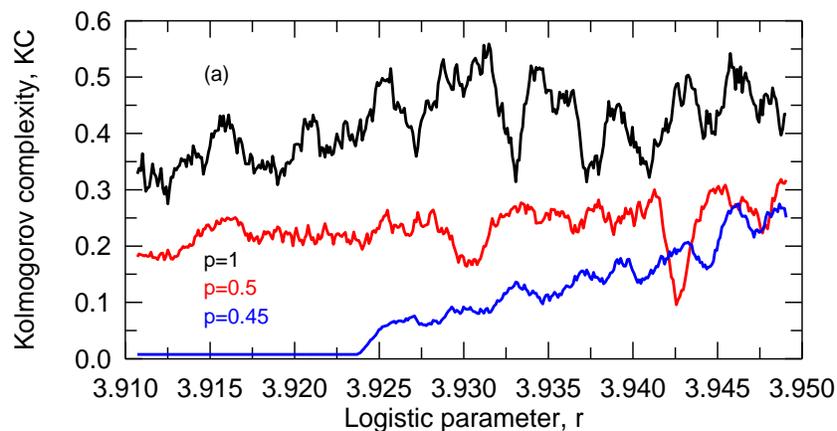
**Figure 3.** Regions of stable and unstable solutions of Eq. (1) for environmental interface temperature, determined by the values of Lyapunov exponent (LE) in dependence of the parameter  $p$  for different values of the logistic parameter  $r$ . LE was calculated for  $r$  ranging from 3.7 to 3.95 by an increment of 0.001 and  $p$  ranging from 0.1 to 1 by an increment of 0.001. Each point was obtained by iterating many times from the initial condition to eliminate transient behavior and then averaging over another 5000 iterations. Initial condition was  $x_0 = 0.25$ .

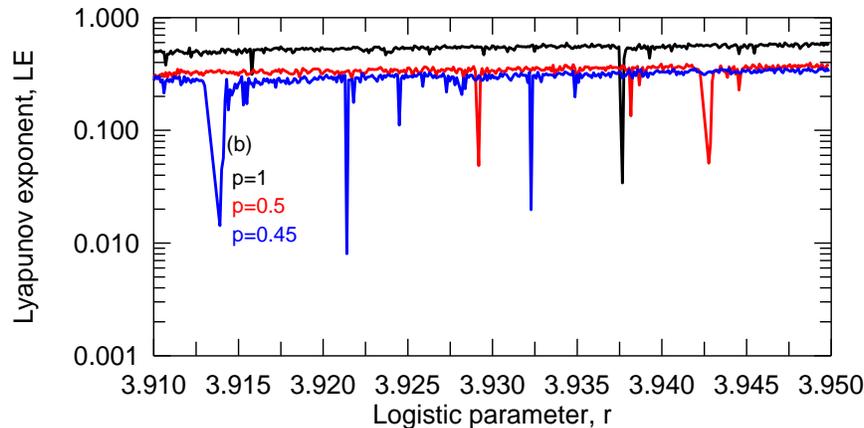
Equation (1) is a nonlinear difference equation that represents time changes of the dimensionless environmental interface temperature respond to the radiation forcing, depending on parameters  $r$  and  $p$  whose solution can exhibit chaotic fluctuations in the considered system because the environmental interface cannot oppose an enormous radiative forcing, suddenly reaching the interface. Therefore, it raises the question whether we can find either domain or domains where physically meaningful solutions exist. Figure 3 depicts unstable solutions (green area) of this equation determined by the values of LE as

a function of  $p$  for different values of the logistic parameter  $r$ . Finally, note that irregularities and chaotic fluctuations in solution of difference equation, describing dynamical systems, can come from the reasons: (i) *numerical*, i.e. because we try to choose appropriate difference equation whose solution is "good" approximation to the solution of the given partial differential equation and (ii) *physical*, i.e. occurrence of chaotic fluctuations of some quantity in the considered system, for example represented by a difference equation of energy balance near to an environmental interface, cannot oppose an enormous amount of energy, suddenly entering system.

#### 4. MODEL PREDICTABILITY AND LYAPUNOV TIME

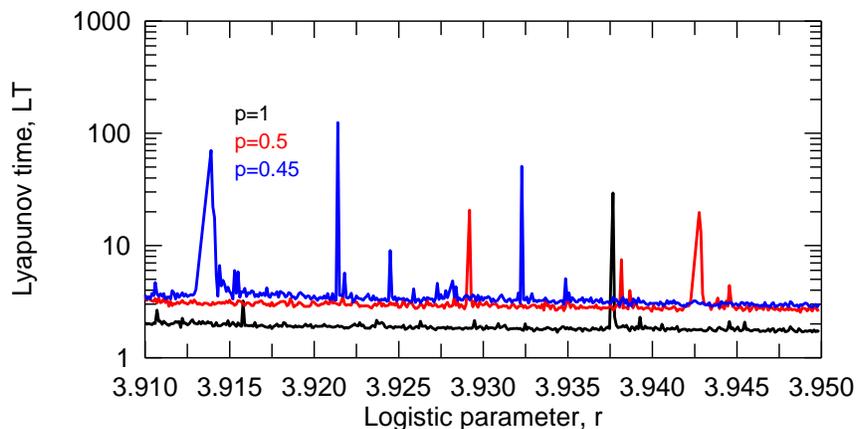
Model *predictability* is the degree to which a correct prediction of a system's state can be made either qualitatively or quantitatively. *Causal determinism* has a strong relationship with predictability. Perfect predictability assumes strict determinism: However, lack of predictability does not necessarily imply lack of determinism, while limitations on predictability could be caused by factors such as a lack of information or excessive randomness. In statistical physics, for example, from the second law of thermodynamics either the equilibrium state can be determined such that a system will evolve to or steady states in dissipative systems can be sometimes also predicted. However, there exists no general rule to predict the time evolution of systems far from equilibrium, e.g. chaotic systems, if they do not approach an equilibrium state. Their predictability usually becomes progressively worse with time where we quantify predictability as the rate of divergence of system trajectories in phase space [for example, Kolmogorov-Sinai entropy, Lyapunov exponents (Boeing, 2016)]. In stochastic analysis a random process is a predictable process if it is possible to know the next state from the present time. In many models, however, the randomness is phenomenon which "spoils" the predictability. For clarity purposes let us underline the following distinction. Chaotic processes should not be confused with random processes since chaos does not imply randomness in any sense. Chaotic processes do not have any kind of distribution like random processes such as Brownian motion that exhibits a Gaussian distribution (Adewumi, 2016). Furthermore, chaotic processes are strictly deterministic. A deterministic system is one where for a given time interval there is only one future state that follows from the current state (Tiberio, 2004). These systems can be described by Ordinary Differential Equations (ODE's). At least three variables are needed for chaos in continuous-time systems as opposed to chaos in discrete systems that requires only a single variable (Shewalo et al., 2012). Conversely to deterministic processes, random processes are attached to some prior probabilities.





**Figure 4.** (a) Kolmogorov complexity (KC) and (b) Lyapunov exponent (LE) of Eq. (1). LE was calculated for ranging from 3.910 to 3.950 by an increment of 0.001 and three different values of  $p$  (0.45, 0.5 and 1). In that calculation each point was obtained by iterating many times from the initial condition to eliminate transient behavior and then averaging over another 5000 iterations. Initial condition was.

To illustrate occurrence of the chaos and randomness in models we employed Eq. (1) with variable values of the parameter  $p$  and the logistic parameter  $r$  that merely simulate changes in modeled physical or any environmental phenomenon, whose evolution is quantified by the Kolmogorov complexity (Mihailovič et al., 2017) and the Lyapunov exponent. The results of simulations are given in Figure 4. Figure 4a depicts evolving of the randomness of Eq. (1) expressed through the KC information measure for three different values of  $p$  (0.45, 0.5 and 1) and the logistic parameter  $r$  ranging from 3.91 to 3.95. Obviously, decrease of this parameter leads to lower complexity (i.e. randomness), which takes the highest values for  $p = 1$ . Figure 4b depicts how the LE evolves in dependence on the aforementioned values of  $p$  and  $r$ . From these figures is seen that randomness of the dynamical system represented by Eq. (1) is not so high (for all three parameters, the KC is less than 0.55), while the LE values lying in the interval (0, 1). If  $LE > 1$ , then the system under analysis is not a chaotic system but rather a stochastic one, and so we cannot make any predictions based on Chaos Theory. Following this criterion considered system is not a stochastic one.



**Figure 5.** Predictability of generalized logistic map [Eq. (1)] given by the Lyapunov time (in time units).

Figure 5 depicts the LE prediction effect for Eq. (1), for different values given by the LT in time units (TU). Simple inspection indicates that the following predictabilities for generalized logistic map [Eq. (1)] were:  $p=0.45$  (around 3 TU in average and extremely 100 TU) and  $p=0.5$  (around 2 TU in average and extremely 11 TU). For  $p=1$  the map had predictability of less than 1 TU (excluding the case  $r=3.936$  when LT was 13 TU). This means that in the interval of the logistic parameter  $r$  ranging from 3.91 to 3.95 Eq. (1) is completely unpredictable already at the level of the time step.

The case  $0 < LE < 1$  then it implies that there is chaos in the system. In that case, one can compute the approximate time limit for which accurate prediction for a chaotic system is a function of LE (Frison and Abarbanel, 1997). Thus, that time (often called *Lyapunov time*) can be calculated as

$$LT = \frac{1}{LE}. \quad (2)$$

If  $LE \rightarrow 0$ , implying that  $LT \rightarrow \infty$  then long-term accurate predictions are possible. In other words this time designates a period, when a certain process (physical, mechanical, quantum, or even biological) moves beyond the bounds of precise (or probabilistic) predictability and enters a chaotic mode.

## 5. CONCLUSIONS

We shortly described (i) definition of the model from the Model Theory point of view and (ii) current situation in the environmental sciences modeling that inherently involves many epistemological questions. It was pointed out that in sciences and accordingly in environmental ones from many reasons modelers ignore nonlinearity of phenomena and processes. We were focused on a *heuristic* technique frequently used in choosing the model in scientific communities, that could be defined as any approach to problem solving that makes use of a practical method not guaranteed to be optimal or "*perfect*", but sufficient either for the immediate goals or until the better approach is reached. In the rest of the study we considered (i) Model choice; (ii) continuous-time versus discrete-time in building the model and (iii) predictability (Lyapunov time) if modelers decide to follow as much as possible the existing nonlinearities in the object that is model. Our considerations were supported by some examples in the modeling of environmental processes.

## ACKNOWLEDGMENTS

This study was realized as a part of the project No. 43007 financed by the Ministry of Education and Science of the Republic of Serbia for the period 2011-2017 and bilateral cooperation project between Serbian and French government under project "*Coupling STICS -LAPS models to improve the representation of crop processes and land-atmosphere interactions (2008-2010)*".

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