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Modeling of Natural Systems: a Physicist Approach

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Abstract

In this paper we discuss, having in mind both students and researchers, the importance of interdisciplinarity in the study of natural systems. In particular, the so called "hard" sciences (physics and chemistry) have been shown to be extremely important in the *explanatory* approach to describe natural systems. Some examples of ecosystems and a list of pertinent scales in their description are presented. Modeling proposals based in the above identified scales, are also mentioned.

1 Introduction

In recent years it became well known the impact of an interdisciplinary approach to deal with the description of natural systems. One may verify that not only researchers interested in classical physical problems like meteorology, but also those interested in water and forest management have adopted this new perspective of scientific approach. The questions concerning natural systems, for long time, have been tackled using only the classical pure *description like* approaches. These systems are now the subject of some *explanatory* studies, where possible mechanisms are suggested, in contrast to the "black" box like studies or simply descriptive approaches.

An important starting point of this new view of natural phenomena was the recognition of the existence of the spatial and temporal *scales*. Presently the starting point of the scientific description of natural systems, involves the identification of the several relevant scales and their associated mechanisms of influence on the system's dynamics. This scale approach can be considered to be initially introduced in an important and difficult problem of physics, namely the study of second order phase transitions [1]. The elimination of several degrees of freedom in approaching the critical temperature of the phase transition [2], suggested a systematic way to describe and identify the dynamics associated to the relevant scales, nowadays not restricted only to thermodynamic phase transitions.

These methods apply also to other physical systems, specified by the relevance of different scales in space and in time (energy) as the Kondo effect [3]. This last problem was exactly solved by K. Wilson [4] after some qualitative ideas introduced by P. W Anderson [5] and also applied to other specific cases [6]. Still more recently, this approach was adopted by J. Luan et al. [7], for identifying and finding the coupling the several spatial/time scales, involved in the description of the operating mechanisms occurring in a tree.

Together with these approaches, the increasing importance of modeling natural systems has been largely recognized in the scientific community [8]. Here one has in mind not only an explanatory point of view, but also, and in some cases very importantly, the *managing* of natural systems, subjected to antrophic (human induced) perturbations.

This text is intended to present an approach for the description of some natural systems, having in view the several different specialists in natural sciences, but mostly directed to bio-scientists and plant physiologists. We then adopt the following way to present these ideas: introduction to the physical descriptions necessary to understand systems involving small space scales. After that, we discuss how to introduce increasing scales together with the system's degree of complexity, in the sense of a large number of interacting degrees of freedom.

2 Multiscale concepts

We start from molecular studies which involve the Angström scale and are described by Quantum Mechanics [9]; these molecular orbital calculations are very useful in the determination of the molecular properties. Other types of calculations, involving clusters, like the discrete variational method(DVM) [10], can also be done for rather simple molecules,

involving a not too large number of different atoms. The advantage of this DVM procedure is to provide, when it applies, an almost first principles calculation of the electronic structure of a relatively simple molecule. Now, if we are considering the atoms constituting the molecule of interest, made of complex atoms, as compared to C or H, the DVM cluster method seems more adequate, because the atomic structure locally is described in more detail as compared to the molecular orbital methods. If one considers organic molecules, the molecular orbital method, which is simpler for these large molecules, seems to be enough precise for a reasonable interpretation of experimental data. We decided to start with the molecular scale because for molecules, the classical quantum mechanical formalism is the adequate one, and corresponds to a *fundamental physics* approach. Nowadays, specific techniques do exist to calculate even very complex molecules, like proteins and enzymes as discussed in [11], [12]. Also some chemical reactions have also been considered [13].

These remarks are motivated by one of our main points, namely the change in scale in passing from molecules to chemical reactions involving complex intermediate configurations. Then one passes to cell scale phenomena, with interactions between light and molecules and enzyme assisted reactions as in the case of photosynthesis (light and dark reactions), which occurs at the leaf level, to later make the crossover to the canopy level [7]. Thus, connecting some of these molecular systems, by including the interactions between them, systems with increasing number of scales (temporal and spatial) [14] can in principle be described at least in a simplified way [15].

Once the electronic structure of the molecule is formally well established, the next natural step for the present description, are the chemical reactions. These are extremely important, if for example one intends to describe *enzymatic reactions*, occurring frequently in natural systems, where the involved spatial scale is again the Angstrom. In some cases, simplified models for the chemical reactions are used, involving parameters , when the microscopic description becomes prohibitively complex. In a more macroscopic level, in leaf's mesophyll, enzyme assisted reactions do exist, which usually are discussed using parametrized model reactions. Here the main parameter is the chemical reaction rate, where even temperature effects may be included using a simple Arrhenius law.

Not only the spatial scales are present and important here, at the molecular level, but also the involved time scales, may have a dominant effect in some cases. Chemical reactions usually lie in the fentosecond time scale as it was shown experimentally in recent works [13]. In summary, the spatial and temporal scales in these chemical reactions are the Angström and the fentosecond. An interesting point is that, in many natural systems, although microscopically involving these scales, their observed macroscopic time scales are very different from the molecular reaction times [13]. Some examples of that, besides photosynthesis, are provided by biochemical reactions occurring in the parts of isolated plants (shoots, leafs and fruits), soil reactions like ion exchange [16] - [19].

Their applications for larger systems, for instance for agricultural purposes, tree stands involving distinct growth rates and different tree species, to end with complex tropical forests, constitute a chain of increasingly complex systems. Examples of these simpler situations have been carefully modeled, but now using an extra ingredient in the dynamics of the system, namely competition for light and nutrients. As it is well known in some cases in physics, the existence of increasing number of degrees of freedom, finishes by

simplifying the global description. This is done by introducing *effective* interactions, where many of these considered scales are in fact included.

The classical examples in well known physical cases are the phase transitions at finite temperatures, using the classical renormalization group technique or its extension to the quantum case for the low temperature range and in some cases, the description of particular fluid dynamics. This is the case of rivers and lakes; the wind direction and its strength along their contour or the cross section for the case of the river, are necessary for modeling the fluid motion, if coupled to the Navier-Stokes equations of classical physics. The case of lakes involves besides these physical approaches, the role of microorganisms in the production of nutrients for fishes and aquatic flora. Lakes and rivers, or in more general cases, the description of hydrology, which together with meteorologic systems are the closest to physical / chemical problems, if one describes the action of micro organisms in terms of the phenomenological chemical reactions.

3 Large scale system: Atmosphere

Historically the only applications of physical theories to natural systems, in the *strictu senso* of the word, were the general circulation models(GCM) of meteorology [20] and its smaller scale mesoscopic description, regional atmosphere modeling system(RAMS), [21]. It should be remembered that even in the case of the GCM or the RAMS simulations, informations about the biosphere are *essential* in order to adequately describe the behavior of the atmosphere. In this case, a modeling of the biosphere must be introduced [22], involving a set of parameters, and well tested models to describe specific parts of the biosphere. If this description is introduced, in order to provide at least an acceptable description, the quality of climate forecasts are visibly increased.

It has been shown long time ago that if one includes only the *atmosphere* and the *sea* dynamics, very *bad* forecasts are obtained. The inclusion of the biosphere properties, even within a simple model description, has been proved to make the results much better, when compared to the available experimental data. Even within this simple modeling of the biosphere, the inclusion of the several relevant scales are to be made. Soil properties and its connection to water and nutrient flow, together with a thermodynamic description of canopy's energy exchange are the fundamental ingredients to be included in the models for these specific systems.

These last remarks provide some examples of the importance of *interconnection* between distinct scientific approaches to describe complex situations, like these atmospheric phenomena, associated to precipitation and as applied for example to hydrology and some applications, involving agricultural systems [22].

The water motion in the soil has two main implications: besides absorption by plants of water dissolved nutrients, one can have also ion exchange in the soil. Clearly this interconnection of approaches is quite important to forest systems, in particular, in the forecast of cloudy days, which directly interferes with photosyntesis performance and thus must be taken adequately into account, if the Carbon balance is to be estimated. To deal with the occurrence of these cloudy days two possibilities are available: one can use experimental meteorological station data or to extract information from general

circulation models.

The last approach is clearly better, since a consistent description is obtained using together the physical descriptions of the atmosphere, including the *associated* modeling for the biosphere, which are parametrized in a sense [19]. Comparison to meteorological experimental results gives a supplementary test of these biosphere models, since the numerical solution of the GCM equations are in present days quite carefully controlled. This biosphere modeling is usually based in a description of some components of the biosphere like trees in forests, rivers and lakes. These models are in general based on resistor/capacitor networks, and may include thermodynamic processes as observed in nature. Again experience obtained in physical electric/electronic networks, can be of extreme usefulness in these cases, and this approach has the name of thermodynamic-networks [23].

4 Forests, crops and plants

A class of natural systems, involving several distinct scales, is provided by trees or more generally forests. The case of crops involves the same collection of scales, but as in the case of forests, the height of the plants introduces a new ingredient, namely the necessary pressure gradient to ensure the nutrient flow and in some cases involve light competition [24]. For the particular case of plants/trees, it has been shown by J. Luan et al. [7] that an adequate scaling, involving several kinds of spatio-temporal scales, can be constructed. This is one of the best examples for natural systems to describe how to eliminate some degrees of freedom, and in so doing, one obtains a receipt to pass from a given spatio temporal scales to larger ones.

Clearly, as in the classical case of phase transitions, that motivated the use of elimination of degrees of freedom, the final dynamics is more complex mathematically to deal with. Some cases require numerical methods like the Monte Carlo technique. In the present case, these calculation difficulties provide, in exchange, a new and deeper view of the several phenomena involved in plants/grasses/forests.

These comments suggest another question concerning the coupling among the several scales as mentioned before. Consider for instance the case of plants. First of all, nutrient transport must be ensured via pressure gradients along the xylem and the phloem, and these nutrients are absorbed from the soil via the roots, helped in some specific cases, by mycorrhiza. This nutrient transport from the soil [25],[26] involves a mesoscopic approach in terms of classical hydrodynamics, describing the water motion in quite distinct layers of the soil , together with possible ion exchange in specific cases. A connection with larger scale phenomena, namely mesoscale RAMS, concerns precipitation which is one of its outputs, together with an evaporation simulation, in some cases modeled within the above resistor/capacitor network.

At the *leaf scale*, the opening of stomata, involves the respiration and water vapor pressure present in the atmosphere, again another output of the RAMS. Taking sun light as one of the fixed external inputs of the model above, except for competition, and the width of the limiting atmosphere, light scattering/absorption should be modeled adequately, as it is made in several works. In some cases one can use an average of cloudy/clear days, as

extracted from meteorological data or from RAMS, and thus estimate the incident radiation of several wave lengths. This procedure is devised mainly to describe photosynthesis performance and leaf light scattering. Again, the simultaneous presence of several scales, including those at the leaf level to describe CO_2 transformation in carbohydrates, necessary to the growth and maintenance of the parts of the plant, the formation of flowers and the several steps of the time evolution of the growth of fruits. Again several scales are involved and in some cases specific models should be developed for each case/scale, for example the case of photosynthesis or plant/fruit growth in terms of the substrate dynamics and in some cases ethylene production.

5 Lakes and rivers

Another branch of active experimental/theoretical work is *limnology*, describing the behavior of lakes and rivers. This is a particularly interesting subject for Brazil, given its diversity of climates and geographic regions. From the more classical physical approach, given the geometric contour of a lake, and specifying for each point its contour, the wind direction and its velocity, a good description of the dynamics of the lake can be obtained. Together with a known lake bottom profile, the solution of the Navier-Stokes equations can be numerically obtained [27]. In principle this model applies for both lakes and rivers, the last case involving the form of river cross section.

The same software, includes a description of the dispersion of dissolved products, occurring at a given region of the lake. These products need not to be only polluents, the same results being also applicable to compounds like nitrogen compounds, generated by the biological action of microorganisms existing in these water ambients.These aspects involve a *mesoscopic* scale for the fluid motion.The presence of phytoplankton and zooplancton requires specific kinds of modeling. These include an estimate of sun light absorption through the water, at least using a phenomenological Beer's model, in view of the description of photosynthetic activities of the phytoplankton. An adequate model for these kind of situations with different interacting systems is the *generalized* reservoir model.

This model is defined as a collection of boxes, with object/product exchange among them. The time derivative of the occupation numbers of any box is determined by the transfer of elements between boxes and to the transfer from/to the outside the system. This model has the same spirit of the chemical reactions mentioned before, in particular, the situations were a controlled input/output of chemical products are included in the usual chemical reactor. Clearly, in such a model, the strengths of the transfer rates may be obtained from other independent models. These should describe the temporal variation of objects/products in terms of the specific dynamics of the subsystems; another possibility is to consider these rates as parameters, fixed by experiment, in the case of descriptive models.

The classical reservoir model incorporates important hypothesis. In its original version one considers only the occupation number of the boxes. The spatial uniformity is always considered in most applications and the validity of this assumption should be carefully tested in each case. In the case of phenomena exhibiting non negligible *space dependence*

of the occupation numbers, transport effects should be included. A classical way of doing that is through the existence of a diffusion term, using for instance Fick's law. This introduces an extra complication, namely the existence of partial differential equations. This implies in the use of specific mathematical techniques, as one has in the case of the modeling of animals migrating along a coast [28] or the classical situations of Turner 's reaction-diffusion equations. This extension needs, for using the reservoir model, the introduction for general cases of a suitable interpretation/justification of the diffusion term.

One possible application of the reservoir model approach is the description of fish webs [29], including several fish species, predator(s) and prey(s), with these fishes imbeded in a larger nutrient reservoir for some non predator fish species. The fishes use, as defenses against predators in some cases, the choice of scapes. Thus, the time dependence of occupation numbers of these special kinds of fish must now include the existence some space dependent preferable sites for the fish to stay, reproduce and feed. Due to the fish motion, a space dependent set of boxes should be introduced. To simplify the model, one may include a position dependent transfer constants, and specific models should be produced for each particular case.

Some specific cases of Iquipari or Grussai lakes, located in the region of the North of Rio de Janeiro, having a connection with the sea, closed with a large sand barrier. In most months of the year, this barrier is kept closed. However the barrier is opened by the fishing community, during special months of the year, to avoid the inconvenient innondations of the community houses, by the increasing of level of the lake. Another reason to open the barrier is to introduce a change in existing fishes, which are captured for food purposes. This problem requires at least a two scale modeling, each one with its specific dynamics. These two models involve: firstly the solution of the classical Navier-Stokes equations for the lake, in presence of wind, inducing water transported substances. The second is a reservoir model to describe phyto and zooplancton dynamics [30], together also with the fish dynamics.

All these models have been adapted to a general reservoir model, with the important assumption of chemical reaction like rate equations. The description of these subsystems, in particular the amounts of P and Mn compounds produced by local organisms, requires an independent model. Note that again a two scale problem is present, and the analysis of experimental data is a critical step to extract the involved rate constants.

6 Final remarks

We hope to have convinced the researchers on several subjects of physico-chemical sciences of the importance of the interdisciplinary approach to the study of natural systems, [31]. Still more importantly, researchers in natural sciences are invited to make contact with this approach which is inspired in many specific techniques developed to deal with physico chemical problems. The exchange of ideas and experiences at this point of the researches in both fields (natural systems and physico chemical), certainly can be extremely fruitful, since both approaches need complementary scientific efforts.

These studied systems, of several kinds exhibiting many degrees of freedom turn out

to be natural candidates to this approach of selecting and eliminating degrees of freedom as one does in a true phase transition problem. The work by Luan et al., has shown how the scale techniques can be useful in an apparently completely distinct natural science problem (description of trees), and this suggests a *new kind of universality*, in this case, universality of the *scale approaches* as applied to the natural system problems.

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