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Octavian Iordache

Modeling Multi-Level Systems

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Understanding Complex Systems

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Modeling Multi-Level Systems

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*...his way was to carry his mind into his laboratory, and literally to make of his
alembics and cucurbits instruments of thought...*

C. S. Peirce

The Fixation of Belief, 1877

Preface

Modeling multi-level complex systems is the object of this book.

Complex systems are assemblies of several subsystems and are characterized by emergent behavior resulting by nonlinear interactions among subsystems for multiple levels of organization.

The complexity of numerous systems is rooted in the existence of many levels of self-organization corresponding to different time and space scales.

There is a need to provide general frameworks able to combine several scales and reality levels of the complex systems in one coherent and transdisciplinary discourse. A challenge for complex systems science and technology is to develop mathematical formalisms and modeling methods able to capture complete systems dynamics by integration of contribution at several hierarchically organized levels. Existing models involve a large number of nonlinear equations, difficult to handle analytically or numerically, and to correlate with real systems behavior. Among the open questions, we mention the definition of relevant parameters and variables to be measured at each scale or level, the study of coupling between different levels, the insufficiency of the algorithmic schema for evolvable or autonomous systems modeling.

The proposed modeling tools for multi-scale and multi-level systems are the polystochastic models, PSM. These characterize systems coming out when several stochastic processes, running at different conditioning levels, are capable to interact with each other, resulting in qualitatively new processes and systems.

Polystochastic models aim to discover and describe new structures and behaviors, which cannot be detected by one level approaches and cannot be reduced to the summation of several levels contributions.

The book is divided in 12 chapters. The chapters 1 to 4 delineate the problems and the methods. The role of multiple levels of reality for different concepts and theories of complexity is highlighted in the first chapter of the book. The relation between levels of reality and categories is emphasized.

Several mathematical methods that have been used in PSM development are briefly presented in chapter 2. This refers to “random systems”, “non-Archimedean analysis”, and “category theory”. Specific concepts as categorification and integrative closure are introduced. Categorical formulation of integrative closure offers the general PSM framework which serves as a flexible guideline for the large variety of research and multi-level modeling problems presented in the book.

Chapter 3 introduces the conventional real-field frame for PSM and some illustrative examples. Chapter 4 leads into the new PSM methodologies. The model categorification method is illustrated. The need of appropriate notions of time and probabilities and of new theoretical concepts is emphasized.

The chapters 5 to 8 are dedicated to case studies relevant to the sciences of nature.

For this part the levels are usually associated to time scales. Chapters 5 and 6 elaborate PSM for mixing and transport in single or multi-compartmental systems while chapter 7 contains a multi-scale study of dispersion and turbulence. Major applications for these chapters range from chemical engineering to pharmacology and environment.

Chapter 8 highlights entropy and entropy production roles for integrative closure conceptual framework. Application concerns entropy production for multi-scale biosystems. Based on different types of causation, new informational entropy criteria are proposed.

The next four chapters, 9 to 12, outline the potential of the proposed multi-level modeling methods for the domain of system sciences. For this part the levels are conceptual knowledge levels or reality levels associated to categories. Chapter 9 establishes the contact of PSM with formal concept analysis. Applications include enumeration of separation flow-sheets, pharmacology, security management for information technology, and failure analysis. Diagrammatic reasoning using existential graphs is presented in chapter 10. The correlations with pragmatism and studies of continuity are emphasized.

Chapter 11 applied evolvable designs of experiments to pharmaceutical pipeline for drug discovery and development, to reliability management systems and failure analysis for printed circuits.

The connection of the presented PSM methodology with some forward-looking research directions for autonomous systems has been outlined by Chapter 12. Delineated case studies refer to autonomous experimentation, case based reasoning, beliefs desires intentions agents, organic and autonomic computing, autonomous animats, viable systems modeling, and multi-level modeling for informational systems.

Necessary elements of non-Archimedean functional analysis and category theory are presented in appendices.

The case studies analyzed in the book, represent a source of inspiration for emerging technologies in their current transition from adaptive toward evolvable and autonomous systems. They joint also recent trends advocating the convergence of disciplines and the need for transdisciplinary research for complexity. The multi-level modeling is in place at the intersection of sciences of matter as chemistry, life sciences, cognitive sciences, engineering and mathematics.

The PSM methodology presented and developed in this book is successfully confronted with an exciting field of major practical interest and a key area for future investigations, the multi-level complexity.

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Abbreviations

CT-category theory

EDOE-evolvable design of experiment

EG-existential graphs

FCA-formal concept analysis

GL-Galois lattice

NA-non-Archimedean

NBIC-nano-bio-info-cogno

PSM-polystochastic model

RS-random systems

RSCC-random systems with complete connections

RTD-residence time distribution

SDG-synthetic differential geometry

SKUP-states, conditions, operators, possibilities

Chapter 1

Introduction

Abstract. A major property of complex systems is their self-structuring in multiple conditioning levels with different spatial and temporal scales.

Multi-scale and multi-level aspects for modern theories and concepts as: dissipative structures, auto-catalytic systems, catastrophes, synergetics, fractals, artificial life, complex adaptive systems, cybernetics, and biomimetic computation are revealed here.

The topic of multi-level structure of reality and its relation to the study of categories is discussed with emphasize on ontology and pragmatism.

1.1 Multi-level Systems

1.1.1 Levels and Complexity

A complex system is described as a structure or a process involving non-linear interactions among many parts and levels, which displays emergent properties. This means that the aggregate system activity is not derivable from the linear summation of the activity of individual components and that novel structure, patterns or properties arise, from interactions among parts.

A survey of the literature indicates that there is no standard definition of a complex or emergent system. However features such as hierarchy of levels, timescales, emergence, unpredictability, interconnectivity, self-organization, self-similarity, collective behavior, evolvability are focused in complexity studies (Adami 2002, Bar-Yam 1999, Kauffman S. 1995, Mainzer 1996).

Complexity is supposed to come from non-linearity and from a large number of elements with many degrees of freedom and many relationships.

A key property of complex systems is their self-structuring in conditioning levels, each of more or less homogeneous characterization.

Spatial and temporal scales may be associated to conditioning levels.

Self-organization will occur when individual independent parts in a complex system interact in a jointly cooperative manner that is also individually appropriate, such as to generate a new level organization.

Complex systems can be studied at different levels of investigation. For example we can study an industrial installation at the level of molecules or at the level of devices interactions. The number of observation levels is finite. The understanding of complexity changes with the domains of application. Some surveys consider that the complexity level has not an absolute meaning, and it is only a relative notion depending on the level of observation or abstraction. These surveys emphasize a facet of complexity as a relative concept which depends both on the task at hand and on the tools available to achieve this task.

For environmental, industrial or pharmacological systems, despite the fact that numerous physical or chemical processes are identified as complex, more of the conventional ones may be operated in regimes where multi-level complexity properties are neglected. For several centuries, physical and chemical sciences made great steps by experimenting and constructing simplified single level models of complex phenomena, deriving properties from the models, and verifying those properties by new experiments. This approach worked because the multi-level complexities ignored in that models were not the essential properties of the phenomena. It does not work when the multi-level complexity becomes the essential characteristic. In an increasing number of cases the multi-level complexity is not transient or atypical, but it is an intrinsic property of that systems.

Several examples will clarify these aspects of complexity.

Consider the moisture dispersion in soil, a first example inspired from environmental studies. Taking into account only particle movements in the inter-particle space of macro pores, simple stochastic process of moisture dispersion will result. This model corresponds to the one level approach. More detailed studies should be concerned about different levels of the real moisture transport process, after macro pores, successive scales of micro pores, restrictions for flow, and so on. In more developed environmental studies a two-state conditional process valued on the set {"wet", "dry"}, should be taken into account on daily and on seasonal scale. The basic physical phenomenon, the moisture migration in soil, arrive to be perceived now as a multi-level complex phenomenon in which many interacting processes, at different levels of organization, evolve in a randomly changing environment. The evolvable multi-scale fluid dispersion ecosystem, self-adapting, self-creating the internal and external restrictions, is the object of the PSM studies.

The next example we will consider is the problem of modeling in industrial multi-scale systems (Fraga et al. 2006). Modeling frameworks should incorporate evolvability in order to selectively manipulate the models and to incorporate details and complexity only in those areas of the models which are critical to provide an adequate solution and remove such details and complexity where it is not. Thus we can imagine a multi-level modeling and simulation capability within which the following hold:

- A model consists of a hierarchy of layers or scales of increasing detail, complexity and sophistication, spanning the entire set of length and time scales from molecules to business chains

- Each layer or scale contains a model definition and a number of parameters
- Each layer accepts parameters from below and calculates the parameters required by the layer above
- Evolvability capabilities such as ontology, languages and agents, may be incorporated at any point to define and modify the models, parameters and solutions

Such multi-level architecture should have a number of capabilities as for instance:

- Should be flexible and extensible
- Should provide a rational and consistent basis for multi-scale models
- Should incorporate external modules, models, codes and be integrated with laboratory and plant systems
- Should allow to the user to indicate fitness for purpose
- Should ensure systems evolvability and autonomy in an environment changing at an ever-increasing rate

As another example we will consider the drug action in pharmacological systems.

The pharmacology seeks to develop a global understanding of the interactions between individual physiology and drug action. To develop such an understanding it is necessary to analyze interactions across and between various scales of organization.

The organisms should be analyzed at the levels of organs, tissues, cells or molecules. Drugs are prescribed at the organism level but exert their effect by interacting with their target at the molecular level.

As observed from these illustrative examples, the complexity of systems arises not only from the number of its components or levels but rather from the way these components are interconnected.

Non-linear interactions between different levels and scales represent a characteristic of complexity. Complex systems differ basically from complicated ones. Systems may outline complexity on both structural and on functional level. Structural complexity increases with the number of interacting subunits, the mutual connectedness among them and the degree of interactions of individual subunits. On a functional level, complexity increases with the minimum length of the algorithm from which one can retrieve the full behavior of the system. Complexity in computing science accommodates a hierarchy of conditioning levels depending on the computational time for computer programs or algorithms. The conditioning levels are determined by the structure as well as the degree of coherent cooperativeness among similar modules of the complex system.

1.1.2 Related Concepts and Theories

Since a universally accepted theory of multi-level complexity does not exist, a brief comparison with related theories sharing similar objectives with PSM, and allowing the study of multi-level systems would be of interest.

Prigogine (1980, 1989) and his group (“Brussels School”) have shown that systems far from equilibrium are able to self-organize in a hierarchical way, in

several levels. The equations of dynamics or of thermodynamics are nonlinear and drive to bifurcations. Non-linearity proves to be necessary but not sufficient for complexity. The emergence of hierarchical levels appears to be one of the possibilities. The complex system organizes itself by jumping from an equilibrium state with few hierarchical levels to another equilibrium state with more levels. By this process the system gets more complex. The resulting structures stable in space and time are called “dissipative structures” (Nicolis and Prigogine 1989). Bénard’s cells and oscillating chemical reactions have been studied as examples of self-organizing processes.

In relation with the above theory, Eigen and Schuster (1979) focused on the origin of life, the domain where chemical self-organization in levels and biological evolution met. The developed concepts were that of “hypercycle”, an auto-catalytic cycle of chemical reactions containing other cycles, and of “quasispecies”, the fuzzy distribution of genotypes characterizing a population of quickly mutating organisms or molecules.

In the theory of so-called “catastrophes”, Thom studied the mathematics of abrupt jumps from a stable steady state to another stable steady state when a control parameter is varying (Thom 1975). For a critical value of the control parameter, the complex system spontaneously jumps from one equilibrium state to another. The process of self-organization by emergence of new levels can be seen as a hierarchical catastrophe by which a system jumps into more and more hierarchical states. For critical values of control parameters, when a new configuration with new levels appears, the system will select it by stochastic mechanisms. Catastrophe theory proposes classifications of the critical behavior of continuous mappings.

Haken (1983) has studied the processes of self-organization by “synergy”, that is by cooperative actions of parts of a system. Results concerning the stability of systems with a large number of degrees of freedom corresponding to different levels associated to timescales and concerning the replacing of fast varying variable by time averages have been pointed in “synergetics” theory. Old structures become unstable and break down by changing control parameters. On the microscopic level the stable modes of the old states are dominated by unstable modes. The main principle in synergetics is the “enslavement principle”. Due to small differences in initial conditions caused by natural fluctuations, one mode will become the master and enslaves all other modes. As a consequence, just a few order parameters are sufficient to describe the complex system. This seems to be the case in the presented here approach where one basic level induce the convergent behavior of the first, second and third levels.

In the last decades the term “fractal” coined by Mandelbrot (1982) was extensively used to describe the class of objects and phenomena, which display scale-invariance and self-similarity for different levels. Fractal identifies structures in which increasing magnification reveals increasing detail and the newly revealed structure looks the same as what one can observe at lower magnification. It was supposed that many structures and features in nature appear as fragmented and manifest properties of scaling and self-similarity. Notable examples are trees and dendrites, humidity pictures, clouds in a solution, amorphous and porous

materials, branched polymers, diffusion-limited aggregates, percolation clusters, and glasses.

General features of the multi-level organized complex stochastic systems with memory have been revealed for “self-organizing systems” theory (Kauffman S. 1995), “stochastic automata” theory, “cellular automata” (Wolfram 1994), in “genetic algorithms” theory (Holland 1996), in “artificial neural network” theory (Carpenter and Grossberg 1987) for adaptive resonance theory, in “artificial life” theory (Langton 1989, 1990), in “complex adaptive systems”, “second order cybernetics” (von Foerster 1981), “autopoiesis” theories (Maturana and Varela 1992), and so on. Multi-level aspects of some of the above enumerated concepts and theories will be briefly presented in what follows.

Kauffman S., (1995) has studied how networks of mutually activating or inhibiting genes can give rise to the differentiation of organs and tissues during embryological development. This led to investigate the properties of multi-level Boolean networks of different sizes and degrees of connectedness. The genetic algorithms introduced by Holland (1996) are parallel, computational representations of the processes of variation, recombination and selection on the basis of fitness that underlay most processes of evolution and adaptation. They have been applied to general problem solving, control and optimization tasks, inductive learning and the modeling of ecological systems.

The “artificial life” approach, tries to develop technological systems such as computer programs and autonomous robots that exhibit life-like properties as for instance, reproduction, swarming, and co-evolution. Based on cellular automata studies, and investigations of self-organized criticality, Langton (1989, 1990) has proposed the general thesis that complex systems emerge and maintain on the edge of chaos, the narrow domain between frozen constancy and chaotic turbulence. The “edge of chaos” idea is a step towards a general definition of multi-level complexity.

Though it shares its subject, the general properties of complex systems across traditional disciplinary boundaries, with cybernetics and systems theory, the theory of “complex adaptive systems” is distinguished by the extensive use of computer simulations as a research tool, and an emphasis on less organized systems, such as ecologies or markets. The “second-order cybernetics” is a theory developed to describe the observed and observing systems (von Foerster 1981). The emphasis on circular, self-referential processes has been continued in Maturana and Varela work on autopoietic systems. The “autopoiesis” that is the self-production denotes the fact that complex systems produce their own components. In that sense they are autonomous or “organizationally closed”. For them the environment is merely a source of perturbations that need to be compensated in order to maintain the system's organization (Maturana and Varela 1992).

The “general systems theory” and the study of complex systems in various fields of human sciences testify the wide variety of hierarchical organizations (Klir 1985, Salthe 1985, Ahl and Allen 1996). It is generally accepted that there is a hierarchy of complexity in nature with more or less highly developed levels of organization. A self-organization realizing the most effects with a restricted

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