



## **The CSS Roadmap for the Science of Complex Systems**

Edited by

Paul Bourgin  
Ecole Polytechnique

David Chavalarias  
Institut des Systèmes Complexes de Paris Ile-de-France

Edith Perrier  
Institut de Recherche pour le Développement

March 2009

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# Roadmap for Complex Systems

This issue of the Complex Systems Roadmap is based on the “Entretiens de Cargèse 2008”, an interdisciplinary brainstorming session organized over one week in 2008, jointly by RNSC, ISC-PIF and IXXI. It capitalizes on the first roadmap and gathers contributions of more than 70 scientists from major French institutions.

The aims of this roadmap is to foster the coordination of the complex systems community on focused objects and questions, as well as to present contributions and challenges in complex systems sciences and complexity science to the public, political and industrial spheres.

## Editorial Committee

- Paul Bourguine - Ecole Polytechnique
- David Chavalarias - Institut des Systèmes Complexes de Paris Ile-de-France
- Edith Perrier - Institut de Recherche pour le Développement

## Contributors

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- Olivier Dauchot - CEA, Commissariat à l'énergie atomique
- François Daviaud - CEA
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- Guillaume Deffuant - Météo-France & U. Paris-Est Cemagref
- Pierre Degond - CNRS
- Jean-Paul Delahaye - LIFL
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- Marie Dutreix - Institut Curie
- Robert Faivre - INRA
- Emmanuel Farge - INSERM-University Paris 7 Denis Diderot
- Patrick Flandrin - CNRS ENS Lyon
- Sara Franceschelli - Paris Jussieu
- Cédric Gaucherel - INRA
- Jean-Pierre Gaudin - IEP
- Michael Ghil - ENS Paris
- Jean-Louis Giavitto - Université Evry
- Francesco Ginelli - Institut des Systèmes Complexes de Paris Ile-de-France
- Vincent Ginot - INRA
- François Houllier - INRA
- Bernard Hubert - INRA
- Pablo Jensen - ENS Lyon
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- Zoi Kapoula - CNRS
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- Olivier Monga - IRD
- Michel Morvan - Ecole normale supérieure de Lyon
- Jean-Pierre Muller - CIRAD
- Ioan Negrutiu - ENS Lyon
- Edith Perrier - IRD
- Nadine Peyreiras - Institut de Neurobiologie CNRS
- Denise Pumain - Université Paris 1
- Ovidiu Radulescu - Université de Rennes 1
- Jean Sallantin - CNRS LIRMM
- Eric Sanchis - Université Toulouse
- Daniel Schertzer - Météo France
- Marc Schoenauer - INRIA

- Michèle Sebag - CNRS
- Adrien Six - Université Pierre et Marie Curie - Paris 6
- Fabien Tarissan - Institut des Systèmes Complexes de Paris Ile-de-France
- Patrick Vincent

# Preamble

In general terms, a “complex system” is any system comprised of a great number of heterogeneous entities, where local interactions among entities create multiple levels of collective structure and organization. Examples include natural systems, ranging from biomolecules and living cells to human social systems and the ecosphere, as well as sophisticated artificial systems such as the Internet, power grid or any large-scale distributed software system. The specificity of complex systems, generally underinvestigated or simply not addressed by traditional science, resides in the *emergence* of non-trivial superstructures that often dominate the system’s behavior and cannot be easily traced back to the properties of the constituent entities. Not only do higher emergent features of complex systems arise from lower-level interactions, but the global patterns that they create affect in turn these lower levels—a feedback loop sometimes called *immergence*. In many cases, complex systems possess striking properties of robustness against various large-scale, multi-dimensional perturbations. They have an inherent capacity to adapt and maintain their stability. Because complexity requires analysis at many different spatial and temporal scales, scientists face radically new challenges when trying to observe complex systems, learning how to describe them effectively, and developing original theories of their behavior and control.

Complex systems demand an interdisciplinary approach. First, because the universal questions that they raise can be expressed under almost the same formulation for widely different objects across a broad spectrum of disciplines—from biology to computer networks to human societies. Second, because the models and methods used to tackle these questions also belong to different disciplines—mainly computer science, mathematics and physics. Last, because standard methods in specialized domains rarely take into account the multiple-level viewpoint so needed in the context of complex systems, and attained only through a more integrated and interdisciplinary approach.

Two main types of interdisciplinary approaches can be envisioned. The first path involves working on an *object* of research that is intrinsically multidisciplinary, for example “cognition”. Here, one poses various questions about the same object from multiple and somewhat disconnected disciplinary viewpoints (neuroscience, psychology, artificial intelligence, etc.)—in contrast to integrated and interdisciplinary. The second path consists in studying the same *question*, for example “synchronization”, in connection with different objects of research in different disciplines (statistical physics, chemistry, biology, electrical engineering, etc.). This second approach establishes the foundations of a true *science* of complex systems. However, the success of these two approaches, which are complementary to one another, is critically dependent on the design of new protocols, new models and new formalisms for the reconstruction of emergent phenomena and dynamics at multiple scales. It is in this joint goal of (a) massive data acquisition on the basis of a set of prior assumptions, and (b) reconstruction and modeling of these data, that the future science of complex systems can develop and thrive. There remains much to do in the theoretical domain in order to build concepts and models able to provide an elegant and meaningful explanation to the so-called “emergent” phenomena that characterize complex systems.

The goal of this roadmap is to identify a set of wide thematic domains for complex systems research over the next five years. Each domain is organized around a specific question or a specific object and proposes a relevant set “grand challenges”, i.e., clearly identifiable

problems whose solution would stimulate significant progress in both theoretical methods and experimental strategies.

**Theoretical questions** are varied. An important aspect is to take into account different levels of organization. In complex systems, individual behavior leads to the emergence of collective organization and behavior at higher levels. These emergent structures in turn influence individual behavior. This raises important questions: what are the various levels of organization and what are their characteristic scales in space and time? How do reciprocal influences operate between the individual and collective behavior? How can we simultaneously study multiple levels of organization, as is often required in problems in biology or social sciences? How can we efficiently characterize emergent structures? How can we understand the changing structures of emergent forms, their robustness or sensitivity to perturbations? Is it more important to study the attractors of a dynamics or families of transient states? How can we understand slow and fast dynamics in an integrated way? What special emergent properties characterize those complex systems that are especially capable of adaptation in changing environments? During such adaptation, individual entities often appear and disappear, creating and destroying links in the graph of their interactions. How can we understand the dynamics of these changing interactions and their relationship to the system's functions?

Questions related to the reconstruction of dynamics from data also play a central role. They include questions related to the epistemic loop (the problem of moving from data to models and back to data, including model-driven data production), which is the source of very hard inverse problems. Other fundamental questions arise around the constitution of databases, or the selection and extraction of stylized facts from distributed and heterogeneous databases, or the deep problem of reconstructing appropriate dynamical models from incomplete, incorrect or redundant data.

Finally, some questions are related to the governance and design of complex systems. “Complex systems engineering” concerns a second class of inverse problems. On the basis of an incomplete reconstruction of dynamics based from data, how can we steer the system's dynamics toward desirable consequences or at least keep the system away inside its viability constraints? How can control be distributed on many distinct hierarchical levels in either a centralized or decentralized way—a so-called “complex control”. Finally, how is it possible to design complex artificial systems, integrating new ways of studying their multilevel control?

All these general questions are detailed in the roadmap. The first questions concern different aspects of emergent phenomena in the context of multiscale systems. The question of reconstructing multiscale dynamics addresses the problem of dealing with incomplete, badly organized and underqualified data sets. Another important aspect to consider is the importance played in complex systems by the reaction to perturbations: it can be weak in certain components or scales of the system and strong in others. These effects, central to the prediction and control of complex systems and models, must be specifically studied. In addition, it is also important to develop both strategies for representing and extracting pertinent parameters and formalisms for modeling morphodynamics. Learning to successfully predict multiscale dynamics raises other important challenges, as the question of being able to go from controlled systems to governed systems in which the control is less centralized and more distributed among hierarchical levels. The last general question addressed in this roadmap concerns the conception of artificial complex systems.

**Grand challenges** for complex systems research draw their inspiration from different kinds of complex phenomena arising from different scientific fields. Their presentation follows the hierarchy of organizational levels of complex systems, either natural, social or artificial. Understanding this hierarchy is itself a primary goal of complex systems science.

In modern physics, the understanding of collective behavior and out-of-equilibrium fluctuations is increasingly important. Biology (in the broad meaning of the word, going from biological macromolecules to ecosystems) is one of the major fields of application where complex behaviors must be tackled. Indeed, the question of gaining an integrated understanding of the different scales of biological systems is probably one of the most difficult and exciting tasks for researchers in the next decade. Before we can hope to integrate a complete hierarchy of living systems, from the bio-macromolecules to ecosystems, each integration between one level and the next has to be studied. The first level concerns the cellular and subcellular spatiotemporal organization. At a higher level, the study of multicellular systems (integrating intracellular dynamics, such as gene regulation networks, with cell-cell signalling and biomechanical interactions) is of great importance, as is the question of the impact of local perturbations in the stability and dynamics of multicellular organizations. Continuing on the way to larger scales raises the question of physiological functions emerging from sets of cells and tissues in their interaction with a given environment. At the highest level, the understanding and control of ecosystems requires integrating interacting living organisms in a given biotope. In the context of human and social sciences, too, the complex systems approach is central (even if currently less developed than biology). One crucial domain to be investigated is learning how the individual cognition of interacting agents leads to social cognition. An important situation requiring particular attention due to its potential societal consequences is related to innovation, its dynamical appearance and diffusion, frequency and coevolution with cognition. Complex systems approaches can also help us gain an integrated understanding of all components, hierarchical levels and time scales in a way that would help moving society toward sustainable development. In the context of globalization and the growing importance of long-distance interactions through a variety of networks, complex systems analysis (including direct observations and simulation experiments) can help us explore a variety of issues related to economic development, social cohesion, or the environment at different geographical scales.

Finally, the fast growing influence of information and communication technologies in our societies and the large number of decentralized networks relying on these new technologies are also in great need of studies and solutions coming from complex systems research. In particular, the trend going from processors to networks leads to the emergence of so-called “ubiquitous intelligence”, which plays an increasing role in how the networks of the future will be designed and managed.

# 1. Questions

## 1.1. Formal epistemology, experimentation, machine learning

**Reporter:** Nicolas Brodu

**Contributors:** Paul Bourguine, Nicolas Brodu, Guillaume Deffuant, Zoi Kapoula, Jean-Pierre Müller, Nadine Peyreiras

**Keywords:** Methodology, tools, computer, experimentation, modeling, validation, machine learning, epistemology, visualization, interaction, functional entity, formalization, phenomenological reconstruction.

### Introduction

Large cohorts of complex entities are more and more available, especially in medicine, in the social sphere and in the environment. The huge size of the data base makes it very difficult to reconstruct their multiscale dynamics through the multiple downward & upward influences. For such a task, the help of a formal epistemology and of computers is indispensable for complex systems scientists, generalizing the kind of open science performed by the high-energy community.

The task of understanding a phenomenon amounts to finding a reasonably precise and concise approximation for that phenomenon and its behavior such that it can be grasped by the human brain. As it is, human intuition cannot handle the intrinsic properties of complex systems unaided. Ideally, optimal formal techniques provide us with candidate concepts and relations, which can then serve as a basis for the human experimental work. When the optimal forms found by the theory do not match the optimal concepts for the human brain, the reason for this discrepancy will itself be the subject of further investigation. Understanding complex systems thus requires defining and implementing a specific formal and applied epistemology. New methods and tools have to be developed to assist experimental design and interpretation for:

- Identifying relevant entities at a given time and space scale.
- Characterizing interactions between entities.
- Assessing and formalizing the system behavior.

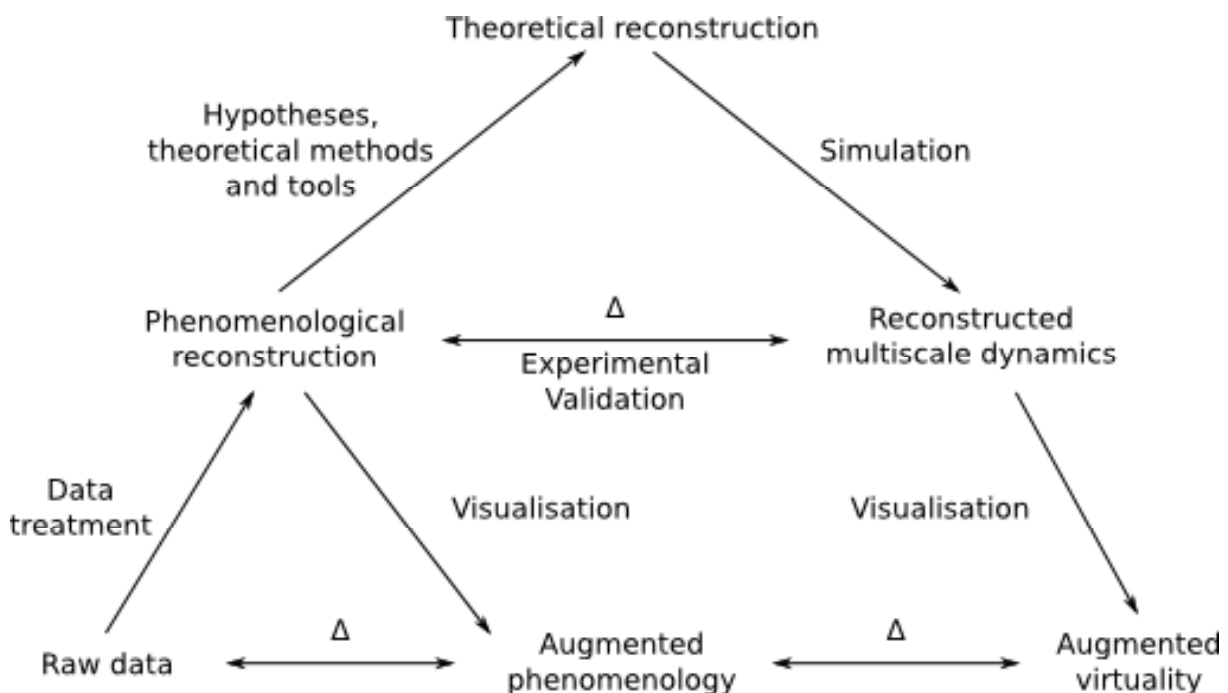
The strategy from experimental design to post hoc data analysis should reconcile the hypothesis- and data-driven approaches by:

- Defining protocols to produce data adequate for the reconstruction of multiscale dynamics.
- Bootstrapping through the simultaneous building of a theoretical framework for further prediction and experimental falsification.
- A functional approach at different levels, leading to the construction of adequate formalisms at these levels. There is no theoretical guarantee that one formal level could then be deducible in any way from another, but this does not matter: Phenomenological reconstruction steps are preferable at each relevant level for the comprehension of the system.

Collecting observations is a necessary part of the methodology. However, there arrives a point at which it is not relevant to go on collecting observations without knowing whether

they are really required for understanding the system behavior. Phenomenological reconstruction leads to data parameterisation and obtained measurements should allow further detection and tracking of transient and recurrent patterns. These features themselves only make sense if they are integrated into a model aiming to validate hypotheses. We expect here to find a model consistent with the observations. The mere fact of building the model necessitates the formalization of hypotheses on the system behavior and underlying processes. Part of the understanding comes from there. More comes from the possibility of validating the model's predictions through experimentation. This last point is depicted on the right-hand side of the graph below.

### Formal & Applied Epistemology



The integration of computer science is an essential component of this epistemology. Computer science should provide:

- Exploratory tools for a data-based approach. Unsupervised learning provides the human with candidate patterns and relations that the unaided human intuition would not grasp. Active machine learning is concerned with determining which experiments are best suited to test a model, which is at the heart of the above epistemology.
- Tools for comparison between the model (hypothesis-driven) and the observations. Supervised learning corresponds to exploring the model parameter space for a good fit to the data. Auto-supervised learning is used when a temporal aspect allows the continuous correction of model predictions with the observed data corresponding to these predictions.

Computer science methods and tools are required in the following steps:

- Human-machine interactions: visualization and interaction with data, ontologies and simulations.
- Building ontology of relevant functional entities at different levels.
- Constructing hypotheses, formalizing relations between entities, designing models.
- Validating the models.

We expect certain fundamental properties from computer science methods and tools:

- Generic tools should be as independent as possible from a logical (interpretation) framework. In particular, because of the varying cultural habits of different disciplines and the specificities of each system, it is preferable to propose a collection of independent and adaptable tools, rather than an integrated environment that would not cover all cases anyway.
- Independence should also apply for the software aspect (for the usage and the evolution and the adaptation of the tools to specific needs). This requires free/libre software as a necessary but not sufficient condition.
- Tools need to be useful for a specialist as well as usable for a non-specialist. For example, by providing domain-specific features that really have an added value for the specialist as extensions (modules, etc.) of the generic tools.
- Readiness for use: The preconditions for the application of the tool should be minimal, the tool should not require a large engineering effort before it can be used.

## **Main Challenges**

### **1. Computer tools for exploration and formalization**

Identifying the computer as an exploration and formalization tool and integrating it into an epistemology of complex systems.

Some research domains currently correspond to this approach and need to be extended. Computational mechanics and its causal state reconstruction is one of these candidate techniques that could possibly automate the phenomenological reconstruction, but there are challenges concerning its real applicability. For example, finding a practical algorithm for the continuous case, or building significant statistical distributions with a limited number of samples (relative to the search space). Statistical complexity can also be considered as a useful exploratory filter to identify the promising zones and interacting entities in the system. Another research domain that could be integrated into the epistemology is the quantification of the generalization capabilities of learning systems (e.g. Vapnik et al.). Automated selection of the most promising hypothesis and/or data instances is the topic of active learning. Its application is particularly straightforward for the exploration of the behavior of dynamical computer models, but more challenging for a multiscale complex system. The problem may be, for instance, to determine response surfaces, leading to a major change of behavior (collapse of an ecosystem, for instance). When the system is in high dimension, the search space is huge and finding the most informative experiments becomes crucial. Some analysis techniques are inherently multiscale (e.g. fractal/multifractal formalisms) and would need to be integrated as well. Dynamical regimes are an essential part of complex systems, where sustained non-stationary and/or transient phenomena maintain the state out of static equilibrium. Some of the existing mathematical and algorithmic tools should be adapted to this dynamic setup and new ones may have to be created specifically. Research is also needed on how to integrate these dynamical aspects directly into the experimental and formal aspects of the above epistemology.

### **2. Computer assisted human interactions**

The computer has become a necessary component of the scientific epistemology, as an extension to the human experimentalist who remains at the center of the loop. Three kinds of interactions involving humans and machines might be considered:

- Machine to human: This corresponds (in particular) to visualization needs. The human sensory system (sight, hearing, etc.) is exceedingly powerful for some tasks, such as

detecting patterns in an image, but quite poor for tasks like visualizing relations in large-dimensional spaces and graphs. Research is needed to provide the human with an adequate representation of a complex system, in a form suitable for the human sensory system.

- Human to machine: The feedback and control that an unaided human can perform on a complex system is similarly limited. For example, when the human is used as the discriminant element for repeated decision-making (e.g. attributing/selecting fitness criteria of model parameters) the bottleneck is the limitation of the human to handle a large amount of such decisions in a time scale corresponding to the optimal execution of the algorithm. As a parallel to the visualization problem, human interaction capabilities on a large-dimensional simulation are relatively poor, especially with conventional devices such as a mouse and keyboard. Finding controls (software or hardware) adapted to the human morphology and limitations is another part of this human/complex system interaction challenge.

- Human to human: The computer should help human communication. For instance, knowledge from domain experts is often lost when non-specialist computer scientists formalize and create the experiments that the experts need. Ideally, the computer should be a tool that enhances - not hampers - cross-disciplinary communication, as well as being directly usable by the experts themselves for designing experiments and models and running simulations. But the use of the computer as a facilitator of human-to-human relations is not limited to interdisciplinary aspects. The computer should become an integrant part of the collaborative process necessary to handle complex systems.

## 1.2. Stochastic and multiscale dynamics, instabilities and robustness

**Reporter:** Daniel Schertzer

**Contributors:** Pierre Baudot, Hughes Berry, François Daviaud, Bérengère Dubrulle, Patrick Flandrin, Cedric Gaucherel, Michael Ghil, Gabriel Lang, Eric Simonet.

**Keywords:** Random dynamical systems, non stationarity, long range/ short range dependence, local/nonlocal interactions, discrete/continuous scaling, cascades, wavelet/multifractal analysis, multiscale modeling and aggregation/disaggregation, pattern recognition, graph dynamics, extremes distribution and large deviations

### Introduction

Hierarchical structures over a wide range of space-time scales are ubiquitous in the geosciences, the environment, physics, biology and socio-economic networks. They are a fundamental building block of our 4D world's complexity. Scale invariance, or scaling for short, is a powerful tool to investigate these structures and to infer properties across scales, instead of dealing with scale-dependent properties. Whereas scaling in time or in space have been investigated in many domains, 4D scaling analysis and modeling are still relatively inchoate, yet indispensable to describe, estimate, understand, simulate and predict the underlying dynamics. Rather complementary to this approach, random dynamical system theory is also a powerful approach for grasping multiscale dynamics. This theory is likely to provide interesting generalizations of what we have learned from deterministic dynamical systems, particularly in the case of bifurcations. Other important domains of investigation are phase transitions, emerging patterns and behaviors which result when we move up in scale in the complex 4D fields.

### Main challenges

#### 1. The cascade paradigm

The idea of structures nested within larger structures, themselves nested within larger structures and so on over a given range of space-time scales has been in physics for some time, and could be traced back to Richardson's book (Weather Prediction by Numerical Processes, 1922) with his humoristic presentation of the paradigm of cascades. This paradigm became widely used well beyond its original framework of atmospheric turbulence, in such fields as ecology, financial physics or high-energy physics. In a very generic manner, a cascade process can be understood as a space-time hierarchy of structures, where interactions with a mother structure are similar in a given manner to those with its daughter structures. This rather corresponds to a cornerstone of multiscale stochastic physics, as well as of complex systems: a system made of its own replicas at different scales.

Cascade models have gradually become well-defined, especially in a scaling framework, i.e. when daughter interactions are a rescaled version of mother ones. A series of exact or rigorous results have been obtained in this framework. This provides a powerful multifractal toolbox to understand, analyse and simulate extremely variable fields over a wide range of scales, instead of simply at a given scale. Multifractal refers to the fact that these fields can be understood as an embedded infinite hierarchy of fractals, e.g. those supporting

field values exceeding a given threshold. These techniques have been applied in many disciplines with apparent success.

However, a number of questions are still open on cascade processes. They include: universality classes, generalized notions of scale, extreme values, predictability and more generally their connection with dynamical systems either deterministic-like (e.g. Navier-Stokes equations) or random (those discussed in the next section). It is certainly important to look closely for their connections with phase transitions, emerging patterns and behaviors that are discussed in the corresponding section. Particular emphasis should be placed on space-time analysis and/or simulations, as discussed in the last section on the general question of space-time scaling.

## 2. Random dynamical systems and stochastic bifurcations

Along with mathematicians' interest in the effects of noise on dynamical systems, physicists have also paid increasing attention to noise effects in the laboratory and in models. The influence of noise on the long-term dynamics often has puzzling nonlocal effects, and no general theory exists at the present time. In this context, L. Arnold and his "Bremen group" have introduced a highly novel and promising approach. Starting in the late 1980s, this group developed new concepts and tools that deal with very general dynamical systems coupled with stochastic processes. The rapidly growing field of random dynamical systems (RDS) provides key geometrical concepts that are clearly appropriate and useful in the context of stochastic modeling.

This geometrically-oriented approach uses ergodic and measure theory in an ingenious manner. Instead of dealing with a phase space  $S$ , it extends this notion to a probability bundle,  $S \times$  probability space, where each fiber represents a realization of the noise. This external noise is parametrized by time through the so-called measure-preserving driving system. This driving system simply "glues" the fibers together so that a genuine notion of flow (cocycle) can be defined. One of the difficulties, even in the case of (deterministic) nonautonomous forcing, is that it is no longer possible to define unambiguously a time-independent forward attractor. This difficulty is overcome using the notion of pullback attractors. Pullback attraction corresponds to the idea that measurements are performed at present time  $t$  in an experiment that was started at some time  $s < t$  in the remote past, and so we can look at the "attracting invariant state" at time  $t$ . These well-defined geometrical objects can be generalized to randomness added to a system and are then called random attractors. Such a random invariant object represents the frozen statistics at time  $t$  when "enough" of the previous history is taken into account, and it evolves with time. In particular, it encodes dynamical phenomena related to synchronization and intermittency of random trajectories.

This recent theory presents several great mathematical challenges, and a more complete theory of stochastic bifurcations and normal forms is still under development. As a matter of fact, one can define two different notions of bifurcation. Firstly, there is the notion of P-bifurcation (P for phenomenological) where, roughly speaking, it corresponds to topological changes in the probability density function (PDF). Secondly, there is the notion of D-bifurcation (D for dynamical) where one considers a bifurcation in the Lyapunov spectrum associated with an invariant Markov measure. In other words, we look at a bifurcation of an invariant measure in a very similar way as we look at the stability of a fixed point in a deterministic autonomous dynamical system. D-bifurcations are indeed used to define the concept of stochastic robustness through the notion of stochastic equivalence. The two types of bifurcation may sometimes, but not always be related, and the link between the two is unclear at the present time. The theory of stochastic normal form is also considerably enriched compared to the deterministic one but is still incomplete and more difficult to establish.

Needless to say, bifurcation theory might be applied to partial differential equations (PDEs) but even proving the existence of a random attractor may appear very difficult.

### **3. Phase transitions, emerging patterns and behavior**

Phase transition is usually associated with the emergence of patterns and collective behavior, for instance due to the divergence of correlation length. Beyond the classical example of glassy systems, these features have been recently observed in shear flows, where the transition from laminar to turbulence occurs discontinuously through gradual increasing of the Reynolds Number. In such a case, the order parameter is the volume fraction occupied by the turbulence that slowly organizes into a band pattern, with a wavelength that is large with respect to any characteristic size of the system.

Similar transition seems to occur in cortical dynamics, when the experimenters increase the forcing of the sensory flow, using spectral or informational measures as an order parameter. When subjected to simple visual input, neuronal processing is almost linear and population activity exhibits localized blob patterns. When subjected to more informational and realistic stimuli, the neuronal processing appears to be highly nonlinear, integrating input over large spatial scales (center-surround interaction) and population patterns become more complex and spatially distributed.

The present challenge is to build a simple stochastic model that accounts for the emerging structures generated by the dynamic and their dependence on the forcing. A more fundamental long-term aim is to catch both glassy and turbulent flow dynamics under such formalism.

A novel approach consists in considering a population of agents that have their own time dynamics and characterizing their collective behavior at different observation scales through gradual aggregation.

The simplest way to aggregate agents is to sum an increasing number of them. When they are identically distributed and independent random variables, the law of large numbers and the central limit theorem apply and the resulting collective evolution is analogous to the individual one. The result does not change when the dependence is short range – this would be the equivalent of the laminar phase. As the spatial dependence becomes long range, the nature of the collective behavior changes (lower rate of convergence, different limit process). The same differences are observed when estimating the density of the law of the variables. By playing with the interaction range, one is therefore able to induce a phase transition.

Another kind of transition is observable if one allows for nonlinear effects in the aggregation process. In such a case, the resulting process may be short-range or long-range dependent, even if the dynamics of the individual are simple (autoregressive short-range dependence in space and time).

A first task is to develop such aggregation methods for simple individual models and to investigate the joint effect of dependence and aggregation process. Examples of applications include geophysical problems, hydrology and hydrography, integrative biology and cognition.

### **4. Space-time scaling in physics and biology**

#### **1) Empirical background**

Systems displaying a hierarchy of structures on a wide range of time and space scales are ubiquitous in physics and biology.

In the geosciences, ‘Stommel diagrams’ displaying life time vs. size of structures (usually in log-log plots) span several orders of magnitude, but a satisfactory explanation of this state of affairs is missing.

In biology, metagenomics have recently been developed to explore microbial biodiversity and evolution by mining urban waste to improve our knowledge of the “tree of life”, but the time structure is far from being reliably estimated.

In computer and social networks, the web is the best-known example, but scale-invariant and small-world networks are encountered everywhere; in this case the temporal aspects have started to be explored, but the connection between the spatial structure and the latter aspects requires further attention.

## **2) State of the art**

a) Taylor’s hypothesis of frozen turbulence (1935), also used in hydrology, is presumably the simplest transformation of time scaling into space scaling. This is obtained by considering that the system is advected with a characteristic velocity.

b) In other cases, the connection between space and time scaling is less evident. As already pointed out, this is the case for computer networks: (space) network topology and (time) computer traffic have been separately studied up to now. Morphogenesis is a research domain that requires the development of space-time scaling analysis.

c) More recently, the comparison of scaling in time vs. scaling in space has been used to determine a scaling time-space anisotropy exponent, also often called a dynamical exponent.

## **3) What is at stake**

a) Why do we need to achieve space-time analysis/modeling?

Basically there is no way to understand dynamics without space and time. For instance, whereas earlier studies of chromosomes were performed only along 1D DNA positions, 4D scaling analysis is required to understand the connection between the chromosome structure and the transcription process.

b) Data analysis

We need to further develop methodologies:

- to perform joint time-space multiscale analysis either for exploratory analysis or for parameter and uncertainty estimations,
- to extract information from heterogeneous and scarce data,
- to carry out 4-D data assimilation taking better account of the multiscale variability of the observed fields,
- for dynamical models in data mining.

c) Modeling and simulations

We also need to further develop methodologies:

- to select the appropriate representation space (e.g. wavelets),
- to define parsimonious and efficient generators,
- to implement stochastic subgrid-scale parametrizations.

## 1.3. Collective behavior in homogeneous and heterogeneous systems

**Reporter:** Francesco Ginelli

**Contributors:** Cyrille Bertelle (Le Havre), Guillaume Beslon (LIRIS, Lyon), David Chavalarias (CREA – ISC-PIF, Paris), Valérie Dagrain (France), François Daviaud (CEA, Saclay), Jean-Paul Delahaye (Lille), Silvia De Monte (CNRS, Paris), Cédric Gaucherel (Montpellier), Jean-Louis Giavitto (IBISC, Evry), Francesco Ginelli (ISC Paris and CEA/Saclay), Christophe Lavelle (Institut Curie, Paris), André Le Bivic (CNRS SDV, Marseille), Jean-Pierre Müller (Montpellier), Francesco d'Ovidio (ENS, Paris), Nadine Peyrieras (CNRS, Gif s/ Yvette), Eric Sanchis (Toulouse), Fabien Tarissan (Ecole Polytechnique)

**Keywords:** Collective dynamics, population diversity, agent-based models, environment heterogeneity, stochastic partial differential equations, reconstruction techniques, mesoscopic description, Lyapunov analysis, phase synchronization

### Introduction

From genetic and social networks to the ecosphere, we face systems composed of many distinct units that display collective behavior on space and time scales clearly separated from those of individual units. Among many others, we can mention cellular movements in tissue formation, flock dynamics, social and economic behavior in human societies, speciation in evolution.

The complexity of such phenomena manifests itself in the non-trivial properties of the collective dynamics - emerging at the global, population level - with respect to the microscopic level dynamics.

Many answers and insights into such phenomena can and have been obtained by analyzing them through the lens of non-linear dynamics and out-of-equilibrium statistical physics. In this framework, the microscopic level is often assumed to consist of identical units.

Heterogeneity is, however, present to varying extents in both real and synthetic populations. Therefore, the existing descriptions also need to encompass variability both at the level of the individual units and at the level of the environment they are embedded in, and to describe the structures that emerge at the population level.

Similarly, homogeneous environment (medium) is a useful approximation for studying collective dynamics. Yet hardly any real, either natural or artificial, environment is homogeneous, thus deeply influencing the structures, dynamics and fates of a population. The variability of the environment applies both on spatial and temporal scales. Examples include filaments and vortices in fluid media, patches and corridors in landscapes, fluctuating resources.

From a methodological point of view, such influences require, at least: the quantification of environmental heterogeneities at different scales; the improvement of the formalization of heterogeneity; the identification of the heterogeneity features that are relevant to the population level and the study of population responses to changes in these heterogeneities.

The question of the generation of heterogeneity of biological systems and its possible requirement for further selecting emergent patterns at different scales is of crucial importance

for our understanding of biological processes. During early steps of embryogenesis in metazoans, cell diversity is generated from the non-homogeneous distribution of sub-cellular components, cell division and cell environment interaction. Cell diversity is required for further functional differentiation. Collective behaviors of cell populations underlying pattern formation should be coupled with cell diversification and differentiation. Both theoretical and experimental aspects of these questions have been almost completely unexplored so far. Finding how molecular and cellular behaviors are coupled in these processes is a main challenge of developmental biology.

Close interaction between nonlinear physicists and biologists, social scientists and computer scientists has proved to be a key ingredient for advances in handling these subjects.

## **Main Challenges**

### **1 Collective dynamics of homogeneous and/or heterogeneous units**

In the past few years, considerable efforts have been devoted to studying and characterizing the emergence of collective phenomena in observation, experiments and at the theoretical level. Examples can be found in a wide range of different systems, from nano-scales to granular matter behavior, neuronal dynamics and social organizations in the animal kingdom (including human societies).

The intrinsic dynamical nature of these phenomena is naturally tackled by the physics of nonlinear systems. As a result, various paths to collective behavior have been identified: phase synchronization in interacting oscillating systems, ordering phase transition in systems of self-propelled agents, self-organization and pattern formation in spatially-extended systems (e.g. ecological systems).

However, we are far from fully understanding the relation between microscopic dynamics and macroscopic properties. For instance, the emergence at the global level of nontrivial coherent dynamics out of unlocked microscopic oscillators, characterized by time scales much shorter than the macroscopic one, still lacks a general theoretical framework. While it has been speculated that transport coefficients can be extracted from the long wavelength components of microscopic linear analysis (Lyapunov analysis), no clear connection has been established so far. Systems of self-propelled units seem to display anomalously large number density fluctuations – unknown in ordinary equilibrium matter and observed experimentally in granular media – but current theoretical models only partially account for such phenomena.

New insights are expected from the intermediate-scale mesoscopic description that bridges the microscopic and macroscopic levels by coarse-graining relevant quantities over appropriate local length and time scales. Due to the importance of fluctuations in out-of-equilibrium phenomena, the resulting partial differential equations (PDEs) are expected to yield stochastic terms, often multiplicative in the coarse-grained fields. The analysis of such stochastic PDEs is an open challenge for physicists and mathematicians alike, both from the numerical and the analytical point of view, but powerful new techniques, such as the non-perturbative renormalization group, promise to shed new light on this subject in the near future.

Although much effort has been devoted so far to systems of homogeneous units, numerous problems of interest deal with systems composed of many different species, such as living systems from single cells to ecosystems. Indeed, fully understanding the emergence of collective phenomena in such systems may require taking into account the interaction between heterogeneous units. Tackling emergence of collective properties in such systems raises numerous questions. To what extent can heterogeneous systems be reduced to

homogeneous ones? In other words, is a wide degree of heterogeneity an irreducible feature of certain systems (for instance complex ecological niches), which cannot be efficiently described in terms of simpler and decoupled few-species models? Are the emergent properties of homogeneous systems conserved in heterogeneous ones, and what are the specific features that arise at the collective level from microscopic heterogeneity? How do new emergent properties relate to previous results obtained in a more homogeneous context? Can the theoretical results acquired on homogeneous contexts be extended towards heterogeneous systems? Can we extend tools developed to model the collective dynamic to take heterogeneity into account (agent-based simulation, for example, can be very naturally extended) or do we have to develop new tools specifically?

At the theoretical level, the study of simple systems composed by coupled oscillators with heterogeneous frequencies may open new insights into more practical systems, while the important role played by synaptic plasticity in neuronal dynamics has long been recognized.

Segregation between different species, on the other hand, can be readily described using heterogeneous agent-based models. On a different scale, cells can be seen as an inhomogeneous fluid. Thus, theoretical results about the behavior of such systems (e.g. phase transition, diffusion in crowded heterogeneous media, etc.) could shed new light on many open questions in molecular and cellular biology, such as the organization of the cell nucleus, diffusion in membranes, signal transduction, regulation of transcription.

Finally, it is worth recalling that the theoretical approach must be developed in parallel with experimental observations. Model studies need to provide results in a form that can be compared and validated with experiments at the quantitative level. In particular, spatial reconstruction techniques – allowing to measure the three-dimensional position and trajectory of each unit inside a large group - are proving increasingly useful for extracting information at the microscopic dynamics level.

## **2. Collective dynamics in heterogeneous environments**

The complexity of collective dynamics is rooted both in individual properties and interactions and in the structure of their environment. Assessing the impact of environmental heterogeneity onto the population is a central challenge in many fields, including biology, geosciences, computer and social sciences.

The complex systems approach should provide a unifying framework for investigating the effect of environmental heterogeneity on population dynamics. In particular, progress is needed in the following directions:

**Multiscale analyses:** observation and measurement of environmental heterogeneity requires new tools for its detection against a noisy background and its analysis at multiple scales. Here, theoretical frameworks are useful to interpret the multiscale heterogeneity behaviors detected. In landscape ecology, for example, the need to capture the scaling sensitivity of mosaic heterogeneity has often been mentioned, while technical tools for this purpose are still lacking. A similar problem arises in plankton studies: turbulence structures the spatial and temporal distribution of the population in scales ranging from centimeters to the oceanic basin, and from minutes to years, but observations currently cover only portions of this range.

**Formalization:** the capture of heterogeneity within models requires the introduction of novel formalization and representation approaches. Equations, algorithms and geometric representations must encompass environmental heterogeneity at different scales and describe and couple the environment with the dynamics of population units. For example, long-range hydrodynamical interactions should be included in models describing the collective motion of bacteria swimming in viscous fluids. Evolution of the vegetal cover has been formalized using

differential equations for continuous diffusion processes or percolation-centered approaches. Yet a mathematical formalization of more discontinuous environments, either in terms of environment heterogeneity or of constituting units, remains to be achieved.

Identification of key environmental features: models cannot include a description of all possible sources of heterogeneity. It will therefore be of key importance to identify the aspects of heterogeneity that are most relevant for the chosen description of the system. Heterogeneity can be examined in terms of concepts such as information, texture, correlation parameters and coherent structures that have to be selected for the collective dynamics under study. For example, landscape structures may exhibit different heterogeneity, depending on the properties influencing the collective dynamics: contrast often highlights barrier effects, while connectivity highlights preferential pathways in the mosaic. In a fluid, transport barriers and mixing regions organize the spatial distribution of tracers; nonlinear methods make it possible to extract such structures from the velocity field and to shed light on the interaction between turbulence and biochemical tracers.

Changing environments: heterogeneity is often not defined once and for all, but can change over the course of time. Such changes can occur on time scales faster than those of the collective dynamics, or manifest themselves as slow drifts in the environmental properties. An example is provided by microbiological populations that live in environments where food availability and temperature are subject to intense fluctuations. Describing the adaptation and evolution of collective behavior requires us to take such fluctuations into account. When the environmental modifications are induced by the population itself, it is the feedback between collective behavior and environmental heterogeneity that shapes the coupled population-environment dynamics, as in the case of the biota-earth interaction in the wake of climate change.

### **3. Emergence of heterogeneity and differentiation processes, dynamical heterogeneity, information diffusion**

From genetic networks to social networks and ecospheres, we face systems that seem to display endogenous heterogeneity: heterogeneity that emerges from the very functioning of the system. Among others, we can mention cell differentiation in ontogeny, social and economic differentiation in human societies and speciation in evolution. The origin and role of this heterogeneity in the viability and maintenance of these large systems is still largely unknown. Yet its importance is recognized in the emergence of topological macro-structures underlying the global functioning of the system. The understanding of the emergence of heterogeneity and its maintenance is thus a challenge for our understanding, management and, possibly, control of complex systems.

From a simple homogeneous structure (multiple copies of the same object or uniform topological space) there are four main types of emergence of heterogeneity, which can be classified in terms of both their Kolmogorov complexity and their logical depth (a measure of "organizational complexity" introduced by Charles Bennett).

(a) Random emergence: noise upon a regular simple structure (random perturbation). One observes an increase in Kolmogorov complexity, but no increase in organizational complexity.

(b) Coordinated or strongly constrained evolution. Example: the duplication of a gene gives two genes, allowing the divergence of their function; varying individuals in a social structure (specialization, new functions, etc.). It is not necessarily associated with a significant increase in Kolmogorov complexity, but with an increase in organizational complexity ("crystallization of a computation").

(c) Mixed emergence: randomness and constraints play a role in the dynamical process of emergence. Examples: whole molecular and genetic modules are re-used and evolve, leading to morphogenetic and functional diversity; speciation by isolation and adaptation to various geographical constraints; several copies of an entity subjected to various conditions diverge by learning or mutual adjustment. There is an increase in both Kolmogorov complexity and organizational complexity.

(d) Emergence by "computation/expression of a pre-existing program". If the "computation" is fast and non-random, there is no increase in Kolmogorov complexity, nor in organizational complexity.

## 1.4. From optimal control to multiscale governance

**Reporter:** Jean-Pierre Müller

**Contributors:** Frédéric Amblard, Jean-Christophe Aude, David Chavalarias, Jean-Philippe Cointet, Valérie Dagrain, Guillaume Deffuant, Pablo Jensen, Maud Loireau, Denise Pumain, Ovidiu Radulescu, Eric Sanchis

**Keywords:** Governance, control, multi-criteria, optimal control, viability, negotiation, multi-level, exploration/exploitation compromise, uncertainty, social acceptability, participation.

### Introduction

When acting on a complex system, institutions in charge of its governance firstly face the problem of defining desired objectives. Often, these objectives must integrate the conflicting interests and points of view of diverse stakeholders at multiple scales. Then, in order to compromise and to decide on policy actions to match the objectives, it is necessary to build an appropriate understanding of the phenomena, often through modeling, and which includes the effect of the potential actions. (Here, we touch again on the general problem of modeling and reconstructing dynamics from data, addressed in another part of the roadmap). Unfortunately, current methods for addressing action policies (reinforcement learning, viability, etc.) are only practically usable for models in state spaces of low dimensionality. Solutions can be sought in two directions: either by extending these methods to multiscale and higher dimensionality dynamics and multi-level actions (e.g. central and decentralized), or by projecting multiscale dynamics in smaller spaces. The use of stylized dynamics, when possible, is another research direction that could open new possibilities for managing good policy actions on complex dynamics. Finally, dynamics are often uncertain and partially unknown, which implies a difficult compromise between exploitation of better known parts of the dynamics and exploration of worse known parts. This problem can be extended to the reformulation of the problem (including the objectives). This framework similarly addresses problems of control and of design.

### Main challenges

- Extending the scope of optimal control
- Projecting complex dynamics into spaces of smaller dimension
- Projecting optimal control into high and multiscale dimension space
- Extending exploration / exploitation compromise to problem reformulation
- Co-adaptation of governance and stakeholders' objectives

#### 1. Extending the scope of optimal control

Current methods of optimal control can deal with uncertain non-linear dynamics, and with flexible definitions of the objectives (in viability theory, for instance), but they are limited by the curse of dimensionality: these methods must sample the state space with a given precision, and this requires an exponential computational power function of the dimensionality of the state space. Extending these methods to spaces of larger dimensions is therefore crucial to enable their use in the context of complex systems.

One potential approach for addressing these questions is to develop weaker frameworks than the optimal control. For instance, the concepts of resilience and viability could provide interesting sources of inspiration in this respect. These concepts require that the system maintains some important functional properties, which is weaker than the traditional objective of optimal control, which aims to maximise a function.

Finally, in some cases, mixing mathematical optimisation of action policies and participatory approaches within an iterative dialog could provide a good compromise between flexibility, social acceptability and rationality. Such approaches would require a specific methodological focus on how to define parts of the problem which can be treated automatically, and how to integrate the results of these optimising algorithms efficiently with other sources within the process of a group decision.

## **2. Projecting complex dynamics into spaces of smaller dimension**

(Sara Franceschelli, Pablo Jensen, Ovidiu Radulescu)

Another possibility to tackle the limits of current control methods is to reduce the dimensionality of complex dynamics (for instance, through the identification of slower parts of the dynamics, the aggregation of the state space, the definition of stylized dynamics and so on). This type of work is also very important in negotiation and formulation processes, in order to give stakeholders intelligible materials from which they can easily express their views. We do not know of reduction approaches directed at the local views of the different stakeholders: such approaches would be very interesting.

Dimensionality reduction applies to both data (information) and models. Statistical techniques based on Principal Component Analysis determine a linear space containing the essential information. They do not apply to non-linear correlation, when projection should lead to curved manifolds. New methods are needed to cover this case as well. Non-linear Independent Components represent one possible direction of research. Classical model reduction techniques are based on separation of time and space scales. We can cite averaging, singular perturbations, calculation of invariant manifolds. These methods are currently used for applications in physics and chemistry and they should be adapted to take into account the specificities of other domains. Furthermore, complex models are only partially specified. For instance, models in biology are qualitative and knowledge of parameters is only partial. Classical model reduction methods start from models that are completely specified (all parameters are known). There is a need for model reduction techniques that can replace numerical information by ordinal information (one parameter is much smaller than others) or other types of qualitative information.

## **3. Projecting optimal control into high and multiscale dimensional space**

(Jean-Christophe Aude, Valérie Dagrain, Guillaume Deffuant, Maud Loireau, Eric Sanchis)

Another possibility is to enlarge optimal control (and any extension beyond optimal control) to high dimensional, multiscale systems. This enlargement should take into account possible distributed actions at different levels, particularly when they are decentralized. Even if the effect of the controls is perfectly known, this perspective is particularly challenging, because in addition to the multi-dimensionality of the system, the control is also in high dimension, with potentially non-linear effects of control coordination. The research should therefore develop new approaches to advance in this direction.

The scope of this approach could be extended to the case where even multiple objectives are defined at different scales. The underlying idea behind this proposition is to introduce the concept of "complex objective". It would probably require the introduction of new formalisms to describe the architecture and links between these multiscale objectives. Since they are described at different levels, current control methods are not suitable for tackling this concept. New research should therefore be undertaken in this field using either centralized or distributed control. The latter method is appealing since it allows to take into account different semantics of control and to act at different scales. This concept raises several questions, including: how to couple and synchronise controllers; how to deal with simultaneous and opposite actions on the system; how to handle the different hierarchical levels; how to mix participation/decision making/optimisation; how to make distributed control with a single global objectives or multiple local objectives or both; how to project the results on multiple perspectives.

#### **4. Extending the exploration/exploitation trade-off to governance analysis**

Decision-makers often face panels of opportunity of actions, among which they have to choose the ones to which they allocate their resources. The outcome and potential success of these opportunities, given their objectives, are often imperfectly known and difficult to evaluate. Therefore, they regularly face a trade-off between exploration of the different available opportunities of action and the exploitation of certain selected opportunities. This trade-off requires experiments at appropriate scales in time and space, and therefore the expenditure of resources, to obtain better knowledge of the value of these opportunities. These expenses must be compared with the potential benefit of such exploration, compared with the mere exploitation of known routines.

In the framework of governance, exploration is necessarily made at a given scale of time and space, whereas governance initiatives are performed within open systems and therefore at several scales of space and time. The challenge is thus to propose methods and tools that can go beyond constraints of exploration and bridge the gap between the results of exploratory experiments and full-scale in vivo implementation of governance actions. These methods would have to take into account the reactive and adaptable nature of the targeted systems, as specified in challenge 1.

#### **5. Co-adaptation of governance and stakeholders' objectives**

In a multi-level context, identifying the stakeholders and territory concerned is a problem in itself. The main problem is to take into account a variety of objectives related to different scales of time and space, which can be more or less reconciled.

The co-existence of different objectives as well as their corresponding potential blueprint, possibly in conflict or in concurrency, raises problems for the management or regulation of the system. Moreover, in some circumstances, the fact that these objectives may evolve according to the evolution of the environment (social context) or may adapt to a dynamical context (Ambient Intelligence) makes the system even more complex to manage or design. The definition of one or several objectives that do not pre-exist and that may emerge is also a key point.

We can focus on two challenges:

##### **5.1 The static dimension: governance in the context of heterogeneity of stakeholders, points of view and interests**

The challenge is to develop models and methodologies to take into account the large heterogeneity of stakeholders' viewpoints and interests, which is reinforced by the entanglement of a large range of space and time scales. Multi-criteria analysis is a starting point for solving these problems, but it must be enlarged in order to incorporate several objectives in parallel, and to include the reformulation process. Moreover, the choice of indicators linked to the objectives or their achievement must include stakeholder participation and must be easy to use. On the other hand, the theoretical consequences of their choice, and particularly the potential biases they may introduce, must be carefully investigated. These tools and methods should also propose criteria to analyse the achievement of the objectives or adequacy to the objectives (any-time evaluation).

## **5.2 The dynamical dimension: evolution of stakeholders' objectives and viewpoints in the governance process**

The challenge is to develop models and methodologies to take into account the feedback loops associated with the self-regulation mechanisms attached to the objectives, as well as the interdependence of particular interests during the governance process. For example, by changing the interaction process, the objectives may change the representations, hence the problem and objective formulation and in return the interaction process. This process becomes even more complex in social settings, where multiple objectives and their coordination occur in the same way, but at the collective level. The time scales of model formation, decision-making and the interaction process itself have to be taken into account.

These aspects of the problem deal with the question of governance, and renew the participative context where co-learning becomes as important as collective negotiation and decision-making. Moreover, the results of the interaction during the governance process can lead to new views of the problem, and possibly new governance objectives (taking into account, for instance, social acceptability) or new structures in the multiscale architecture of the governance organizations.

## 1.5. Reconstruction of multiscale dynamics, emergence and immergence processes

**Contributors:** David Chavalarias, Jean-Philippe Cointet, Paul Bourguine, Michel Morvan, Nadine Peyrieras.

**Keywords:** Micro-macro reconstruction, multi-level experimental protocol, emergence, immergence, dynamical systems, multiscale systems.

### Reconstruction of multiscale dynamics and emergence and immergence processes

The data related to complex systems are most often incomplete and difficult to exploit because they are limited to a single level, i.e. refer to observations made on particular scales of space and time. Gathering data effectively first requires the definition of common concepts and pertinent variables for models at each level. Another important problem is obtaining unified and coherent representations for integrating different levels of organization as to predict the dynamics of the complete system. This goal can be achieved by defining pertinent variables at each level of organization, i.e. at different time (slow/fast) and spatial (macro/micro) scales, their relationships, and how they are coupled together in models that describe the dynamics at each level. The challenge is to make explicit integration functions from micro to macro levels (emergence functions) and from micro to macro levels (immergence functions).

#### Grand challenges:

1. Building common and pertinent references in the life sciences.
2. Achieving coherence in the modeling of complex systems.
3. Development of mathematical and computer formalisms for modeling multi-level and multiscales systems.

#### 1. Building common and pertinent references in the life sciences

The data relating to complex systems are often incomplete and therefore difficult to exploit. A main challenge is to find common methods to collect data at different levels of observation, which are coherent and compatible in the sense that they can be used in order to integrate a multi-level (multiscale) system. Thus, it is necessary to find multiscale models that allow researches to define pertinent experimental variables at each level and to achieve a common reference frame with data reproducibility in the different levels of organization of the complete system.

#### 2. Achieving coherence in the modeling of complex systems

The goal is to find coherence in the definition of variables and models used at each level of the hierarchical system and to make compatible the models that are used to describe the dynamics at each hierarchical level of organization at given time and space scales.

As a first step, one must ensure that natural constraints are taken into account and that fundamental laws are verified at each level of description (definition of pertinent species, symmetry laws, physical laws, conservation laws and so on). The next step is to connect the

description and models used at each level to those at other levels:  
(i) Modeling the dynamics at microscopic levels can be useful for defining boundaries for global variables and even to obtain correct interpretations for global variables.  
(ii) Modeling the dynamics at macroscopic levels can be helpful for defining local functions and variables governing microscopic dynamics.

### **3. Development of mathematical and computer formalisms for modeling multi-level and multiscale systems.**

The complexity of natural and social systems stems from the existence of several levels of organization corresponding to different time and space scales. A major challenge of complex systems science is to develop formalisms and modeling methods in order to rebuild the complete system by integration of its hierarchical multiscale levels. This goal can be achieved by defining emergence and immergence functions and integrating intra-level (horizontal) and inter-level (vertical) couplings.

Mathematical models used to describe the dynamics of natural and social systems involve a large number of coupled variables at different space and time scales. These models are in general nonlinear and difficult to handle analytically. Therefore, it is crucial to develop mathematical methods that allow one to build a reduced system governing a few global variables at a macroscopic level, i.e. at a slow time scales and long spatial scales.

Among open questions, we mention the definition of pertinent variables at each level of organization and their relationships. It is also necessary to obtain emergence (resp. immergence) functions that allow analysis to jump from a microscopic (resp. macroscopic) level to a macroscopic (resp. microscopic) level, to study the coupling between the different levels and therefore the effects of a change at one level of a hierarchy on the dynamics at others.

Methods based on the separation of time scales already allow the aggregation of variables and are used in mathematical modeling for integrating different hierarchical levels. However, such multi-level modeling methods need to be extended to computer modeling and particularly to IBM (Individual Based Models) and constitute a very promising research theme. Also, the comparison of multi-level models to experimental data obtained at different levels remains also a major challenge which has to be investigated in parallel to the development of mathematical and computer modeling methodologies for multi-level systems.

## 1.6. Designing artificial complex systems

**Reporter:** René Doursat

**Contributors:** Jean-Christophe Aude, Sofiane Ben Amor, Marc Bui, René Doursat, Jean-François Mangin, Jean Sallantin

**Keywords:** artificial assistants, virtual simulations, functional modeling and regulation, bio-inspiration, autonomous and evolutionary systems.

### Designing Artificial Complex Systems

Modeling and simulation are crucial complementary tools in the exploration of complex systems. The recent and fast-growing development of complex systems research in many scientific fields, along with the strong interdisciplinary interactions that it created, was greatly stimulated by the striking advances in computer networks and high-performance calculation. Information and communication technologies represent today a major tool of investigation in complex systems science, often replacing analytic and phenomenological approaches in the study of emergent behavior. In return, information technologies also benefit from complex system research. Artificial complex systems can be created to analyze, model and regulate natural complex systems. Conversely, new and emergent technologies can find inspiration from natural complex systems, whether physical, biological or social.

### Grand Challenges:

1. Using artificial complex systems for the understanding and regulation of natural complex systems
2. Finding inspiration in natural complex systems for the design of artificial complex systems
3. Building hybrid complex systems.

### 1. Using artificial complex systems for the understanding and regulation of natural complex systems

Natural complex systems (NCS) include systems found in nature (pattern formation, biological organisms, ecosphere, etc) but also systems spontaneously originating from human activity (cities, economy, transportation, etc.) A key application of artificial complex systems (ACS) is to assist the description, generation and support of these NCS. One major challenge is to design and develop systems that can carry out a methodical exploration and/or regulation of NCS. In particular, ACS design can complement human collective intelligence by integrating different levels of expertise and harmonize or manage contradictions in collaborative works. Such artificial systems can be based on structures and functioning principles different from the natural systems they observe. An ACS could serve to regulate, schedule, repair or modify the NCS. The execution of ACS can be asynchronous and separate from the NCS, or it can be integrated with it.

### Examples:

- Reconstructing the topology of neural connections in the brain by means of neuro-imagery and artificial vision based on a distributed architecture

- Observation of interest groups and interaction networks on the Internet (forums, blogs, instant messaging) through software agents
- Airflight dynamics and network

## **2. Finding inspiration in natural complex systems for the design of artificial complex systems**

In order to create technological systems that are autonomous, robust and adaptive, new engineering approaches must draw inspiration from NCS. For example, in computer security, systems able to mimic the biological immune system can provide useful solutions against continuously evolving attacks on computer networks. These ACS are built upon intrinsically distributed, self-organizing and evolutionary entities. They reproduce the original behavior and organizational principles that are found in NCS but have no equivalent in traditional technical design. In some domains, biology could even replace physics at the foundation of new engineering principles.

NCS provide rich sources of ideas in the development of decentralized systems that can display robustness, modularity, and autonomy in dynamically changing environments (i.e., “ubiquitous computing”, “ambient intelligence”). ACS should be able to reproduce the dual principles of cooperation and competition that are observed in NCS.

On the other hand, bio-inspired artificial design is not constrained by any fidelity to the original NCS. Computer and technological innovation can free designers from experimental data or real examples of functioning mechanisms. Examples include neural networks inspired by neuroscience and genetic algorithms by Darwinian evolution. ACS created this way can also play a heuristic exploratory role for NCS. Engineering inventions allow us to better understand, even predict the natural phenomena that inspired them.

### **Examples:**

- Neuro-inspired artificial intelligence and robotics
- Collective optimization and swarm intelligence inspired from social animal behavior
- Evolutionary robotics
- Intelligent materials, auto-assembling materials, and morphogenetic engineering (nanotechnologies)
- Ambient intelligence
- Computer security inspired by immune systems or social interactions

## **3. Design of Hybrid Complex Systems**

The rapid dissemination of computing devices and systems in our society (cellphones, PDAs, etc.) and the intricacy and profusion of their interconnections constitute a major case of hybrid or “techno-social” complex systems. Such systems can be studied as complex communities combining natural and artificial agents. Users can instruct machines, themselves capable of autonomous learning and adaptation to their environment.

# 2. Objects

## 2.1. Complex matter

**Reporter:** F. Daviaud

**Contributors:** G. Biroli, D. Bonamy, E. Bouchaud, O. Dauchot, F. Daviaud, M. Dubois, B. Dubrulle, F. Ladieu, D. L'Hôte.

**Keywords:** Glassy dynamics, slow relaxations, frustration and disorder, collective behaviors, out-of-equilibrium and nonlinear systems, self-organization, turbulence, dynamo action, fracture

### Introduction

The field of complex and non-equilibrium systems is currently driven by a large body of new experiments and theoretical ideas in various branches of physics, from condensed matter physics up to ultra-cold atomic physics and biology. Beyond their apparent diversity, these systems share a common characteristic: the emergence of complex collective behaviors from the interaction of elementary components. Glassy dynamics, out-of-equilibrium systems, the emergence of self-organized or self-assembled structures, criticality, percolating systems, domain wall propagation and pinning of elastic walls, nonlinear systems, turbulence and fracture propagation are some subjects of complex matter that can be addressed only with the tools developed for the study of systems of interacting entities. Understanding these phenomena also requires the development of new theoretical methods in statistical physics and the design of new types of experiments.

### Main challenges

1. Non-equilibrium statistical physics
2. Damage and fracture of heterogeneous materials
3. Glassy dynamics: glasses, spin glasses and granular media
4. Bifurcations in turbulence: from dynamo action to slow dynamics

### 1. Non-equilibrium statistical physics

The long lasting interest for non-equilibrium phenomena has recently experienced a noticeable revival, because of the concomitant development of novel theoretical ideas (especially on the symmetries of non-equilibrium fluctuations) and of new areas of applications, ranging from many examples in condensed matter physics to other branches of physics (heavy ion collisions, the early universe) and to other sciences, including biology (manipulations of single molecules). Non-equilibrium phenomena also play an important part in many of the interdisciplinary applications of statistical physics (modeling the collective behavior of animals, or social and economic agents).

A physical system may be out of equilibrium for either of the following two reasons:

Slow dynamics. The microscopic dynamics of the system is reversible, so that the system possesses a bona fide equilibrium state. The dynamics of some of the degrees of freedom is however too slow for these variables to equilibrate within the duration of the

experiment. The system is therefore in a slowly evolving non-equilibrium state for a very long time (forever in some model systems). The characteristic features of this regime of non-equilibrium relaxation, including the violation of the fluctuation dissipation theorem, have been the subject of intense activity over the last decade. This kind of situation is commonly referred to as aging (see the part on glassy dynamics).

Driven dynamics. The dynamics of the system is not reversible, usually because of some macroscopic driving caused by external forces. For instance, an electric field induces a non-zero current across the system. This driving violates the reversibility of the underlying stochastic dynamics. The system reaches a non-equilibrium stationary state, where it stays forever. There are also systems (at least model systems) where the lack of reversibility lies entirely at the microscopic level, and does not rely on any macroscopic external driving. The paradigm of such a situation is the celebrated voter model.

One of the most salient advances of the last decade has been the discovery of a whole series of general results concerning the symmetries of spontaneous fluctuations in non-equilibrium states. These theorems, associated with names such as Gallavotti, Cohen, Evans and Jarzynski, have been applied and/or tested in many circumstances, both by theory and experiment.

Most recent efforts in this area have been devoted to interacting particle systems. This broad class of stochastic systems is commonly used to model a wide range of non-equilibrium phenomena (chemical reactions, ionic conduction, transport in biological systems, traffic and granular flows). Many interacting particle systems can be investigated by analytical methods, whereas some of them have even been solved exactly.

Although the usual formalism of equilibrium statistical physics does not apply to out-of-equilibrium systems, it is now well-known that many of the tools developed in equilibrium can be used out-of-equilibrium. This is in particular the case for the framework of critical behavior, scale invariance, finite-size scaling, which have provided (largely numerical) evidence for universality in non-equilibrium systems. It is possible to investigate systems in which the non-equilibrium character stems not from the presence of gradients imposed, for instance, by boundary reservoirs, but because of the breaking of microreversibility - that is to say, time-reversal invariance - at the level of the microscopic dynamics in the bulk.

A large part of the research activity on non-equilibrium statistical physics is also centred on the various phase transitions observed in many contexts. Indeed, many non-equilibrium situations can be mapped onto each other, revealing a degree of universality going well beyond the boundaries of any particular field: for example, self-organized criticality in stochastic (toy) sand piles has been shown to be equivalent to linear interface depinning on random media, as well as to a particular class of absorbing phase transitions in reaction-diffusion models. Another prominent example is the jamming transition which bridges the fields of granular media and glassy materials. It has been studied experimentally thanks to a model experiment consisting in a sheared layer of metallic disks. Synchronization and dynamical scaling are, likewise, very general phenomena which can be related to each other and to the general problem of understanding universality out of equilibrium.

## **2. Damage and fracture of heterogeneous materials**

To understand the interrelation between microstructure and mechanical properties has been one of the major goals of materials science over the past few decades. Quantitative predictive models are even more necessary when extreme conditions – in terms of temperature, environment or irradiation, for example – or long-time behavior are considered. While some properties, such as elastic moduli, are well approximated by the average of the properties of the various microstructural components, none of the properties related to fracture

– elongation, stress to failure, fracture toughness –follow such an easy rule, mostly: (i) because of the high stress gradient in the vicinity of a crack tip, and (ii) because, as the more brittle elements of microstructure break first, one is dealing with extreme statistics. As a result, there is no way that a material can be replaced by an “effective equivalent” medium in the vicinity of a crack tip. This has several major consequences:

### **Size effects in material failure**

In brittle materials, for example, cracks initiate on the weakest elements of the microstructures. As a result, toughness and life-time display extreme statistics (Weibull law, Gumbel law), the understanding of which requires approaches based on nonlinear and statistical physics (percolation theory, random fuse models, etc.).

### **Crack growth in heterogeneous materials**

Crack propagation is the fundamental mechanism leading to material failure. While continuum elastic theory allows the precise description of crack propagation in homogeneous brittle materials, we are still far from understanding the case of heterogeneous media. In such materials, crack growth often displays a jerky dynamics, with sudden jumps spanning over a broad range of length-scales. This is also suggested from the acoustic emission accompanying the failure of various materials and - at much larger scale - the seismic activity associated with earthquakes. This intermittent “crackling” dynamics cannot be captured by standard continuum theory. Furthermore, growing cracks create a structure of their own. Such roughness generation has been shown to exhibit universal morphological features, independent of both the material and the loading conditions, reminiscent of interface growth problems. This suggests that some approaches issued from statistical physics may succeed in describing the failure of heterogeneous materials. Let us finally add that the mechanisms become significantly more complex when the crack growth velocity increases and becomes comparable to the sound velocity, as in impact or fragmentation problems, for instance.

### **Plastic deformation in glassy materials**

Because of high stress enhancement at crack tips, fracture is generally accompanied by irreversible deformations, even in the most brittle amorphous materials. While the physical origin of these irreversible deformations is now well understood in metallic materials, it remains mysterious in amorphous materials like oxide glasses, ceramics or polymers, where dislocations cannot be defined.

## **3. Glassy dynamics**

### **Glasses**

The physics of glasses concerns not only the glasses used in everyday life (silicates), but a whole set of physical systems such as molecular glasses, polymers, colloids, emulsions, foams, Coulomb glasses, dense assemblies of grains, etc. Understanding the formation of these amorphous systems, the so-called glass transition, and their out-of-equilibrium behavior is a challenge which has resisted a substantial research effort in condensed matter physics over the last decades. This problem is of interest to several fields from statistical mechanics and soft matter to material sciences and biophysics. Several fundamental open questions emerge: is the freezing due to a true underlying phase transition, or is it a mere crossover with

little universality in the driving mechanism? What is the physical mechanism responsible for the slowing down of the dynamics and glassiness? What is the origin of the aging, rejuvenation and memory effects? What are the common concepts that emerge to describe the various systems evoked above, and what remains specific to each of them?

Interestingly, however, evidence has mounted recently that the viscous slowing down of super-cooled liquids and other amorphous systems might be related to the existence of genuine phase transitions of a very singular nature. Contrary to usual phase transitions, the dynamics of glass-formers dramatically slows down with nearly no changes in structural properties. We are only just beginning to understand the nature of the amorphous long-range order that sets in at the glass transition, the analogies with spin-glasses and their physically observable consequences. One of the most interesting consequences of these ideas is the existence of dynamical heterogeneities (DH), which have been discovered to be (in the space-time domain) the counterpart of critical fluctuations in standard phase transitions. Intuitively, as the glass transition is approached, increasingly larger regions of the material have to move simultaneously to allow flow, leading to intermittent dynamics, both in space and in time. The existence of an underlying phase transition and of dynamical heterogeneities should significantly influence the rheological and aging behaviors of these materials, which are indeed quite different from those of simple liquids and solids. As a consequence, progress in the understanding of glassy dynamics should trigger several technological advances. An important example where the peculiar properties of glasses are used in technology is the stocking of nuclear waste.

From an experimental point of view, the major challenges for the future have been transformed not only because progress in the domain has led to radically new questions, but also because new experimental techniques now allow to investigate physical systems at a microscopic scale. In previous decades the, focus was mainly on the behavior of timescales and of global properties. New challenges for the years to come are: i) To study the local dynamical properties in order to unveil what changes in the way molecules evolve and interact makes the dynamics glassy, in particular why the relaxation time of supercooled liquids increases by more than 14 orders of magnitude in a small temperature window; ii) To provide direct and quantitative evidence that glassy dynamics is (or is not) related to an underlying phase transition; iii) To study the nature of the dynamical heterogeneities (correlation between their size and their time evolution, fractal dimensions, etc.); iv) To investigate the nature of the out-of-equilibrium properties of glasses, such as violation of the fluctuation-dissipation theorem, intermittence, etc.

From a theoretical point of view, the major challenge is to construct and develop the correct microscopic theory of glassy dynamics. This will consist both in unveiling the underlying physical mechanisms that give rise to slow and glassy dynamics and in obtaining a quantitative theory that can be compared to experiments. The main focus will again be on local dynamic properties, their associated length-scale and their relation to the growing timescales and the global properties of glassy dynamics.

## **Spin glasses**

The expression "spin glasses" was invented to describe certain metallic alloys of a non-magnetic metal with few, randomly substituted, magnetic impurities. Experimental evidences were obtained for a low temperature phase characterized by a non-periodic freezing of the magnetic moments with a very slow and strongly history-dependent response to external perturbations. Basic fundamental ingredients of spin glasses are disorder and frustration. The frustration consists in the fact that the energy of all the pairs of spins cannot be minimized simultaneously. The theoretical analysis of spin glasses lead to the celebrated

Edwards-Anderson model: classical spins on the sites of a regular lattice with random interactions between nearest-neighbor spins. This has led to many developments over the years, and the concepts developed for this problem have found applications in many other fields, from structural glasses and granular media to problems in computer science (error correction codes, stochastic optimization, neural networks, etc.).

The program of developing a field theory of spin glasses is extremely hard, with steady, slow progress. The theory is not yet able to make precise predictions in three dimensions. Numerical simulations face several difficulties: we cannot equilibrate samples of more than a few thousand spins, the simulation must be repeated for a large number of disorder samples (due to non-self-averaging), and the finite size corrections decay very slowly.

Spin glasses also constitute an exceptionally convenient laboratory frame for experimental investigations of glassy dynamics. The dependence of their dynamical response on the waiting time (aging effect) is a widespread phenomenon observed in very different physical systems such as polymers and structural glasses, disordered dielectrics, colloids and gels, foams, friction contacts, etc.

### **Granular Media close to the Jamming transition**

Common experience indicates that as the volume fraction of hard grains is increased beyond a certain point, the system jams, stops flowing and is able to support mechanical stresses. The dynamical behavior of granular media close to the 'jamming transition' is very similar to that of liquids close to the glass transition. Indeed, granular media close to jamming display a similar dramatic slowing-down of the dynamics as well as other glassy features like aging and memory effect. One of the main features of the dynamics in glass-forming systems is what is usually called the cage effect, which accounts for the different relaxation mechanisms: at short times, any given particle is trapped in a confined area by its neighbors, which form the so-called effective cage, leading to a slow dynamics; at sufficiently long times, the particle manages to leave its cage, so that it is able to diffuse through the sample by successive cage changes, resulting in a faster relaxation. Contrary to standard critical slowing down, this slow glassy dynamics does not seem related to a growing static local order. For glass-formers it has been proposed instead that the relaxation becomes strongly heterogeneous and dynamic correlations build up when approaching the glass transition. The existence of such a growing dynamic correlation length is very important in revealing some kind of criticality associated with the glass transition.

One can, for example, study the dynamics of a bi-disperse monolayer of disks under two different mechanical forcings, i.e. cyclic shear and horizontal vibrations. In the first case, a "microscopic" confirmation of the above similarity has been obtained and the second can provide the experimental evidence of a simultaneous divergence of length and time scales precisely at the volume fraction for which the system loses rigidity (jamming transition).

## **4. Bifurcations in turbulence: from dynamo action to slow dynamics**

**Dynamo action** Dynamo action consists in the emergence of a magnetic field through the motion of an electrically conducting fluid. It is believed to be at the origin of the magnetic fields of planets and most astrophysical objects. One of the most striking features of the Earth's dynamo, revealed by paleomagnetic studies, is the observation of irregular reversals of the polarity of its dipole field. A lot of work has been devoted to this problem, both theoretically and numerically, but the range of parameters relevant for natural objects are out of reach of numerical simulations for a long time to come, in particular because of turbulence.

In industrial dynamos, the path of the electrical currents and the geometry of the (solid) rotors are completely prescribed. As this cannot be the case for planets and stars, experiments aimed at studying dynamos in the laboratory have evolved towards relaxing these constraints. The experiments in Riga and Karlsruhe showed in 2000 that fluid dynamos could be generated by organizing favourable sodium flows, but the dynamo fields had simple time dynamics. The search for more complex dynamics, such as exhibited by natural objects, has motivated most teams working on the dynamo problem to design experiments with less constrained flows and a higher level of turbulence. In 2006, the von Karman sodium experiment (VKS) was the first to show regimes where a statistically stationary dynamo self-generates in a fully turbulent flow. It then evidenced other dynamical regimes for the first time, including irregular reversals - as in the Earth - and periodic oscillations -as in the Sun.

These complex regimes, involving a strong coupling between hydrodynamic and MHD, need to be studied in detail. In particular, they reveal that although the dynamo magnetic field is generated by the turbulent fluctuations, it behaves as a dynamical system with a few degrees of freedom.

Theoretical predictions regarding the influence of turbulence on the mean-flow dynamo threshold are scarce. Small velocity fluctuations produce little impact on the dynamo threshold. Predictions for arbitrary fluctuation amplitudes can be reached by considering the turbulent dynamo as an instability (driven by the mean flow) in the presence of a multiplicative noise (turbulent fluctuations). In this context, fluctuations can favor or impede the magnetic field growth, depending on their intensity or correlation time. We can use direct and stochastic numerical simulations of the MHD equations to explore the influence of turbulence on the dynamo threshold.

**Bifurcations in turbulence** At high Reynolds numbers, some systems undergo a turbulent bifurcation between different mean topologies. Moreover, this turbulent bifurcation can conserve memory of the system history. These aspects of the turbulent bifurcation recall classical properties of bifurcation of low-dimensionality systems, but the bifurcation dynamics is really different, probably because of the presence of very large turbulent fluctuations. Future studies will be concerned with the universal relevance of the concept of multistability in average along time of states of highly fluctuating systems and by the transitions between these states (e.g. magnetic inversions of the Earth, climate changes between glacial and interglacial cycles). The slow dynamics of turbulent systems, in the case where exchanges of stability can be observed for some global quantities or some averaged properties of the flow, should also be studied, and an attempt made to construct nonlinear or stochastic models of those transitions.

In the case of turbulent flows with symmetry, it is also possible to construct a statistical mechanics, and develop a thermodynamical approach to the equilibrium states of axisymmetric flows at some fixed coarse-grained scale. This allows the definition of a mixing entropy and derivation of Gibbs states of the problem by a procedure of maximization of the mixing entropy under constraints of conservation of the global quantities. From the Gibbs state, one can define general identities defining the equilibrium states, as well as relations between the equilibrium states and their fluctuations. This thermodynamics should be tested in turbulent flows, e.g. von Karman flow. Effective temperatures can be measured and preliminary results show that they depend on the considered variable, as in other out-of-equilibrium systems (glass). Finally, we can derive a parameterization of inviscid mixing to describe the dynamics of the system at the coarse-grained scale. The corresponding equations have been numerically implemented and can be used as a new subgrid scale model of turbulence.

## 2.2. From molecules to organisms

**Reporter:** Christophe Lavelle

**Contributors:** Pierre Baudot (Paris), Hugues Berry (INRIA, Saclay), Guillaume Beslon (IXXI-LIRIS, Lyon), Yves Burnod (INSERM, Paris), Jean-Louis Giavitto (IBISC, Evry), Francesco Ginelli (CEA, Saclay), Zoi Kapoula (CNRS, Paris), Christophe Lavelle (Institut Curie, Paris), André Le Bivic (CNRS SDV, Marseille), Nadine Peyrieras (CNRS, Gif s/ Yvette), Ovidiu Radulescu (IRMAR, Rennes), Adrien Six (UPMC, Paris)

**Keywords:** Systems biology and integrative biology, stability, fluctuation, noise and robustness, physiopathology, biological networks, computational biology, multiscaling in biological systems.

### Introduction

Biological investigations are expected to provide knowledge that is transferred at some point to clinical research for handling human physiopathology. This means that we hope to cure better, if possible, or at least to understand better. Yet it is now becoming ever more clear that better understanding will arise from an integrative view of biological systems. We thus need to develop this integrative grasp further and to transfer the knowledge acquired in this framework to clinical research. This interdisciplinary approach should provide novel insights into physiology and pathology.

After a brief presentation of the general aims and concepts discussed in this topic, 4 main challenges are listed and detailed.

How investigations should be driven in biology is a matter of debate. Should they be data-driven, object-driven or hypothesis-driven? Do we at least agree about the aim of deciphering the causality underlying biological processes? Do we expect models to bring insights and knowledge about the behavior of biological systems, through predictions?

Recent advances in functional genomics and in the study of complex diseases (such as cancer, autoimmunity or infectious diseases, mitochondrial diseases, metabolic syndrome) have shown the necessity of an alternative way of thinking in biology, in which pathology and physiology are considered to result from interactions between many processes at various scales. A new scientific field has emerged from this need. Systems biology is the study of gene, protein, and biochemical reaction networks and cell population dynamics, considered as dynamical systems. It explores the biological properties resulting from the interaction of many components, investigating processes at different scales and achieving their integration. Complex systems provide a conceptual framework and effective tools to unravel emergent and immergent features from molecules to organisms and vice versa. The latter, described as immergence, microemergence or downward causation, means that some macro-level constraints are expected to cascade back onto micro-levels. Both emergent and immergent properties should be derived from the multiscale reconstruction of data recorded at the appropriate spatial and temporal scales, to be defined through new types of protocols. We expect to find generic processes (design patterns for computer science) that apply from an upper to a lower organizational level and vice versa and that allow their coupling e.g. synchronisation, reinforcement, amplification, inhibition, achieved through basic processes such as signalling through molecular interactions, diffusion, vesicular transport, ionic transport, electric coupling, biomechanical coupling and regulation of molecules and macromolecules characteristic features (including their concentrations).

Complex systems are almost always multiscaled both in time (typically femtoseconds in chemical reactions, seconds in metabolism processes, days to months in cells, years in an living organism) and space (typically nanometers for molecular structures, micrometers for supramolecular assemblies, organelles and cells, centimeters for tissues and organs, meters for organisms). Finding the pertinent space & time scales for experimentation and modeling is a major issue. As a result of evolutionary opportunism (biological tinkering), multiscale space & time correlation is not a priori given. Classical approaches (biochemistry, cellular and molecular biology, behavioral and cognitive studies, etc.) usually have their “preferred” scale by default, mainly due to the fact that protocols and experiments are often designed to work only at a specific scale. This makes back and forth interactions between different scales in observations, experimentations, models and simulations a very exciting transdisciplinary challenge.

Variation in biological systems raises the issue of an average, typical or representative behavior. Addressing this point requires characterizing and measuring variability and fluctuations at the molecular, single cell, cell population and physiological levels. The origin, time and space scales, control and functional significance of fluctuations in biological systems are largely unknown. Their functional significance might be approached through their multiscale transmission and possible amplification, reduction/damping or role in mediating bifurcations.

Obviously, understanding will not arise from a one-to-one description and modeling of organisms (virtual cell, virtual organism) but rather from the correct identification of which components are relevant for a given problem and the reconstruction of the mechanisms involved. Such a reconstruction should use mathematical and physical tools, some borrowed from out-of-equilibrium thermodynamics and dynamical systems. New tools will also be required to answer specific questions of biology. Ultimately, injecting systemic vision and using complex systems principles and conceptual frameworks for a better understanding of human physio-pathology could lead to novel differential diagnosis and improve medical care.

## **Main challenges**

1. Fluctuations and noise in biological systems
2. Stability in biology
3. Multiscaling
4. Human physiopathology

### **1. Fluctuations and noise in biological systems**

Modern biology has developed with the idea of average behaviors or individuals. But this conceptual framework has recently been challenged by empirical observation. Quantitative measurements within living single cells have revealed extensive variability and fluctuation of cellular dynamics between different cells or between different times within the same cell. These observations open a new conceptual framework in biology, in which noise must be fully considered if we are to understand biological systems, while the classical framework tended to consider it as a mere measurement error or as "simple" thermodynamic fluctuations that have to be reduced by cells.

This new point of view raises many questions and both practical and theoretical issues that will probably deeply modify our understanding of biological systems. However, to tackle these questions, we need to develop a complete scientific program from precise measurements through to analysis of the origin and functional role of stochasticity in biological systems, at all of their time and space scales. Among the main breakthroughs, we need to:

- Improve the technology for quantitative measurements of noise and fluctuations in single cells, cell populations, tissues, organs and individuals. In particular, it will be necessary to identify the characteristic times at each level of organization and the most appropriate experimental indicators.
- Identify the mechanisms by which noise and fluctuations arise in biological systems. In particular, what are the modalities of multiscale transmission of fluctuations? Are fluctuations amplified or reduced/damped from one scale to the others? Are they important with respect to bifurcations in the organism/cell fate?
- Understand the functional significance of fluctuations in the different biological systems. For instance, it has been proposed that fluctuations can enhance the robustness of living beings. However, other processes can be envisaged (e.g. stochastic resonance, increased signaling rates, cell differentiation, evolution, etc.). Such a functional significance supposes that biological systems are able to control the level of noise.
- Delineate possible mechanisms by which biological systems may control their level of fluctuation (negative/positive feedback loops in biochemical networks, neuronal adaptation in cortical networks, adaptive mutations and mutation hotspots, regulations and networks in the immune system).
- Question the meaning of usual averaging processes in experimental biology. In the case of biochemical networks, can data gathered on cell populations be used to infer the actual network in a given single cell. Similar issues arise in the case of connectivity structures of cortical networks and cell lineage reconstruction.

These issues can be addressed in various biological systems including (but not limited to):

- Transcription and regulation networks: it is now clear that the transcriptional activity of the cell is highly stochastic. Some of the molecular causes of this stochasticity have been identified. However, the precise origin and regulation mechanisms of this stochasticity are still to be discovered. This will first require the development of adequate measurement methodologies to enable us to quantify these fluctuations at different time scales in single cells.
- Neurons and neuronal networks: the on-going activity of cortical circuits is a spontaneous activity generated by the recurrent nature of these networks. It has long been considered a mere noise added to the environmental signals. However, more recent studies have proposed a real functional role in which ongoing activity could facilitate signal spreading and be implicated in adaptive processes. Inhibitory effects have been shown to reduce variability at both the single-cell and population level.
- Diversity of the immune system: The immune system is characterized by diversity at different levels. Lymphocyte receptor diversity, populations of effectors and regulators, cell-population dynamics, cell selection and competition, migration through the whole organism are the result of somewhat stochastic or selection mechanisms whose impact in the overall efficiency of the system needs to be further characterized.
- Uncontrolled variability is often accused of being a source of major perturbations in the fate of organisms. Examples can be found in the process of aging, cancer, autoimmunity, infections or degenerative diseases. Yet the precise influence of noise is still open to debate. In particular, one point is to determine to what extent degenerative processes are a consequence of noise accumulation, a consequence of a variation of the noise properties or a consequence of rare stochastic events.
- Variability at the genetic level is the major engine of evolution. But genetic variability may be indirectly regulated according to the spatio-temporal characteristics of the environment (selection for robustness, selection for evolvability). Moreover, clonal

Concerning the modeling of fluctuations, several mathematical and physical tools exist, but these need to be improved. Thus:

- Stochastic models are largely used in molecular systems biology. The simulation algorithms (Gillespie algorithm) use the Delbrück-Bartholomay-Rényi representation of biochemical kinetics as jump Markov processes. In order to improve the performance of these methods (which are costly in time) several approximate schemes have been proposed, for instance the approximation of Poisson variables by Gaussians (tau-leap method). Hybrid approximations are more appropriate when the processes are multiscale and these approximations could be developed by combining averaging and the law of large numbers. In certain simple cases, the master equation can be exactly solved.
- It is also interesting to transfer ideas from statistical physics to biology. For instance, fluctuation theorems, which concern the occurrence of out-of-equilibrium fluctuations in heat exchanges with the surrounding environment and work theorems, concerning thermodynamic fluctuations in small systems close to equilibrium, could be applied to characterize fluctuations in gene networks, DNA transcription processes and the unfolding of biomolecules.

## 2. Stability in biology

We encounter various definitions depending on the phenomenon, the model or the community proposing the concept. Homeostasis in relation to metabolic control, the Red Queen concept in evolution describing continuous development to sustain stable fitness in a changing environment, robustness in systems biology referring to insensitivity with respect to perturbations, canalization and attractors in developmental biology and ecology are all forms of stability.

### Main Challenges

1) Biological systems are only stable on a finite horizon, constantly submitted to perturbations (intrinsic or extrinsic). The notion of steady state, or more generally attractor, has to be revisited. We need new mathematical concepts to describe this type of stability.

o Finite-time stability is a concept that can be used to define stability in the case when the system is known to operate or to preserve its structure unchanged over a finite time. We are interested in the conditions under which the system's variables remain within finite bounds. Can we extend such formalism to other properties (oscillations, optimal biomass production, etc.)?

o Finite time stability depends on the existence of subsystems with different relaxation times. It is thus important to develop methods allowing to estimate the largest relaxation time of subsystems. For compound systems, how can we relate the relaxation times of the elements to that of the system?

o The notion of resilience is also a generalization of stability that is particularly appealing in this context. Indeed, it focuses on the ability to restore or maintain important functions when submitted to perturbations. The formalizations of this concept, founded on dynamical system

properties (measure of attraction basin sizes), or even on viability theory (cost to return into a viability kernel) should become more operational to favor a wider diffusion.

2) The functioning of multicellular organisms occurs at the level of the population, not of the individual cell. Furthermore, the stability of a cell population (tissue) is generally different from that of the individual cell. For example, cells extracted from tumours can reverse to normal activity when injected into healthy tissue. In this context, how can we define and study the stability of a population in relation to the stability of individuals? In addition, the same relation should be considered in the context of a developing organism taking into account differentiation and organogenesis. These processes are examples of symmetry-breaking, and we would like to determine whether symmetry arguments can be used in the study of stability properties.

3) Systems biology studies robustness as an important organizing principle of biological systems. As pointed out by H. Kitano, cancer is a robust system with some points of fragility. Thus, finding treatments and cures for diseases may consist in determining the fragility points of a robust system. In order to answer this question, we need good models, new mathematical theories and computer tools to analyse properties of models and new experimental techniques to quantify robustness.

4) Complexity and stability. Models of an organ and models relating several organs to each other imply the collaborative representation of the components. Similarly, gene regulation models gather numerous molecular details. In the modeling process, we should be able to zoom in and out between various levels of complexity. Stable properties of the system could be those that are common to several levels of complexity. More generally, is there a connexion between stability and complexity?

### **3. Multiscaling**

Biological processes involve events occurring at many different time and space scales. The hierarchy of these scales enters the scene only because it corresponds to our subjective views of the system, usually based on our various discrete experimental accesses. Multiscale approaches drawn from theoretical physics have been developed essentially in an unidirectional (bottom-up) way, to integrate parameters and mechanisms at a given scale into effective, and hopefully reduced, descriptions at higher scales. However, lower-scale properties are directly coupled with properties of the higher scales (e.g. 3D chromosome distribution in the nucleus partly governs gene expression, which itself participates in nuclear architecture). The very complexity of living systems and biological functions lies partly in the presence of these bidirectional feedbacks between higher and lower scales that have become established over the course of evolution. Self-consistent or iterative “up-and-down” approaches therefore need to be introduced to account for the strong interconnections between the levels and ensuing circular causal schemes.

#### **Multiscaling vs. self-scaling**

To properly account for the behavior of a biological system, a multiscale approach should jointly tackle all the scales, with no way to skip a priori any microscopic details or macroscopic assemblies. Obviously, such modeling would rapidly reach a high level of complexity, and would ultimately be intractable. This limitation on multiscale descriptions imposes a drastic change in the paradigm underlying the modeling of biological systems.

To reduce the complexity level, it has been proposed (Lavelle/Benecke/Lesne) to devise models taking the biological function as a starting point and continuing guideline, driving both integrated modeling and supervised data analysis to parallel the biological functional logic. Decomposition is achieved by dissecting its logic and implementation into basic processes. These elementary processes involve features at different scales and are already integrated in their formulation. More generally, such a decomposition results in “self-scaled” functional modules, independent of the arbitrary description or observation scale. As function-dependent representations are inherently multiscale in nature, and the function cannot be discontinuous, this paradigm-transition consequently requires a scale-continuous model. Scale-continuous descriptions may at first sight look prohibitively complex and non-realistic; however, when such a scale-continuous model is constructed in the context of a function-dependent representation, the dimensionality of the variable-vector to be considered collapses.

### **Emergence vs. immergence**

Modeling of biological systems is required to develop formalisms in order to rebuild the complete system by integration of its hierarchical multiscale levels. It can be achieved by defining "micro to macro" (emergence) and "macro to micro" (immergence, microemergence or downward causation) functions and integrating intra-level (horizontal) and inter-level (vertical) couplings. The definition of pertinent variables at each level of organization and their relations is necessary to obtain emergence (resp. immergence) functions that allow analysis to jump from a microscopic (resp. macroscopic) level to a macroscopic (resp. microscopic) level. Emergence and immergence phenomena are well-known in biology, such as the links between the structure topology of tissues and cell behavior. But these causal relationships are difficult to decypher, mainly because the scales at which they occur are not necessarily those at which observations and experiments are done.

- How should we select relevant space and time scales in our experiments/models/theories (selfscaling rather than exhaustive multiscaling)? Can we correlate multiscale in time and space (at least in some instances) in this sorting?
- How can we perform multiscale reconstruction from data recorded at different scales? On which spatial and temporal scales will the model/simulation obtained be valid?

## **4. Human physiopathology and animal models**

Human physio-pathology creates uncertainties with constantly moving frontiers between disciplinary fields, for example, neurology, neurosciences, psychiatry, immunology, cardiovascular, metabolism, endocrinology. Human patho-physiology is characterized by progressive dysfunction and deterioration at multiple space and time scales with non-linear interactions between physiological/biological functions, cognition, emotions, and social consequences. Problems can result initially from local conflict between internal and external signals (e.g. dizziness), but this conflict can expand, diffuse and create additional loops with multiple pathogenic reciprocal interactions. Functional problems could be primary or secondary effects of spontaneous adaptive mechanisms aiming to counter primary injury and dysfunction, and it is important to dissociate them.

Two main challenges are:

- to apply complex system principles and theoretical frameworks to the design of experimental studies and the analysis of data at different scales (neurological,

- to search for cross-correlations and interactions in order to obtain new insights into pathogenic primary or secondary mechanisms. This could lead to new, more sensitive differential diagnostic tools, but also to better medical care or functional re-adaptation. There is a need to go beyond a limited multi-disciplinarity of parallel different approaches and use complex systems tools to cross data from different fields and gain further insight.

This issue concerns the whole internal & general medicine, immunology, neuroscience, psychiatry, geriatrics, pediatrics, functional re-education, public health, and complex systems science. Examples of functional problems, some of which have no measurable organic basis are: vertigo - dizziness and equilibrium problems and fear of falling in the elderly, isolated hearing loss, tinnitus, learning problems – dyslexia, but also neuro-degenerative diseases, types of dementia, Lewy-Body and Alzheimer. What causes the switch from physiological auditory noise to perceived unwanted signal in the case of tinnitus in the absence of neuro-otological findings?

Major questions include the significance of instantaneous fluctuations of measurements (physiologic, behavioral, e.g. in the case of dementia) in relation to pathophysiology and progressive degeneration of cortical-subcortical circuits. Other examples could be given in immunology: time and space (lymphoid tissues), analysis of the functionalities of the immune system in physiological (ontogeny to aging, gestation) and pathological conditions (cancer, autoimmunity, infections), and interactions with other biological systems such as the nervous, endocrine, metabolic systems. This is based on dynamics analysis of fluid lymphoid cell populations, quantification and identification of phenotype and functions, repertoires, genomics and proteomics.

## 2.3. Physiological functions

**Contributors:** Catherine Christophe, Christophe Lecerf, Nadine Peyrieras, Jean Sallantin.

**Keywords:** in vivo observation and measurement devices, spatial and temporal multiscale observations, subcellular and supra-cellular functions, organism-environment interaction, ontogenesis, physiological disorders.

### Physiological functions

Physiological functions result from the integration of cells, tissues and organ properties in the context of the whole organism interacting with its environment. A complex system approach of physiological functions should lead to an iterated cycle combining relevant measurements and experimentation, modeling and simulation. Such a goal requires building multimodal investigation devices for simultaneous in vivo recording at different spatial and temporal scales of relevant parameters as well as designing theoretical methods and tools for appropriate modeling and computer simulation.

#### Grand challenges:

1. Integrating multimodal measurements and observations of physiological activities at different spatial and temporal scales.
2. Characterizing the contextual features determining the onset of operation, maintenance and modulation of a physiological function.
3. Investigating the relationship between the ontogenesis of a physiological function and its potential disorders.

Expected results include the design of new investigation devices and theoretical methods and tools for observing, modeling, understanding and then possibly controlling physiological functions.

#### 1. Integrating multimodal measurements and observations of physiological activities at different spatial and temporal scales.

An integrated observation of sub cellular and supra cellular processes requires to either:  
(i) Translate in the same spatial and temporal referential heterogenous data recorded in the same organism but at different moments, or  
(ii) Design new devices capable of simultaneously recording multimodal data.

The first goal can be achieved through available methods going from spatio-temporal matching to data fusion. These methods are limited by recalibration problems and errors (whatever the rigid or elastic transformations applied).

The second option would be a real breakthrough providing a generation of totally new instrumentation offering instantaneously access to essential structural and dynamic variables (chemical, electrical, mechanical, etc.) at all relevant spatio temporal scales. This trend can be exemplified by macroscopic data acquisition in medical imaging with optical-PET and PET-CT devices and, for vital physiological variables, by ambulatory integrated sensors providing real-time patient state tracking in a normal environment. In the domain of vegetal biology, phenotypic plant platforms lead to the observation of flow from roots to leaves at different time scales.

Integrating such synchronous, multimodal, multiscale observations in relevant models should provide a good basis for the reconstruction of physiological functions.

## **2. Characterizing the contextual features determining the onset of operation, maintenance and modulation of a physiological function.**

The objective is here to view the function as an integration of subfunctions that should be investigated from different perspectives or using perturbative and comparative approaches.

Different factors or conditions such as resting versus moving, diet-nutrition, training, can influence and move the system towards new functioning modes.

Comparative physiology provides a way to study the conservation or divergence of physiological functions. This approach is relevant for respiration and locomotion in the animal kingdom as well as for fruit maturation in the field of vegetal biology.

Physiological functions should be characterized through the extraction of high-level variables, i.e. “thermodynamics variables”? along the lines of allometry (i.e. preservation of characteristics over the size variations). More generally, we should be able to define invariants (or invariant relationships) attached to physiological functions and the conditions for their conservation.

## **3. Investigating the relationship between the ontogenesis of a physiological function and its potential disorders.**

Physiological functions should be explored through their set up during ontogenesis, maturation and maintenance during growth, adulthood and ageing. The dynamical behavior of physiological functions should be explored as well during pathological events.

Examples:

- Heart embryology: progressive formation of anatomical structures and functional patterns with ill-posed problems related to the partial observations at our disposal (i.e interpolation of highly structurally variable objects from the architectonic viewpoint, installation of nodal tissue functions or sinusal electric waves, etc.)
- Schizophrenia: effects on the highest cognitive levels of the modifications induced by the disease at the level of more elementary neurological functions

## 2.4. Ecosystemic complexity

**Contributors:** Olivier Barreteau, Paul Bourguine, David Chavalarias, Cédric Gauchere, François Houllier, Ioan Negrutiu, Nadine Peyrieras

**Keywords:** ecological dynamics, adaptation and evolution, ecological services, multi-functionality of the ecosystems, integration of data, coupling of models, space-time dynamics, multiscale models, disturbance and resilience, stability and dynamic transition, emerging behavior, feedback and retroaction, functional organization.

### **Ecosystemic complexity**

Defined as the close association of an abiotic environment and a collection of living organisms, an ecosystem, essentially, is characterized by a great number of physicochemical factors and biological entities which interact with each other. The multiplicity and diversity of these interactions as well as the fact that they involve a vast range of levels of organization of Life and a broad spectrum of space and temporal scales justify the expression of “ecosystemic complexity”?

Moreover, the ecosystems, be they natural, managed or artificial, are subjected to “perturbations”? (e.g. natural hazards or biotic and abiotic stresses) and deliver many and diversified commercial and non-commercial products and “services”? To identify, qualify, formalize and quantify these modes of disturbance and these products and services define research topics that refer, according to cases, to the sciences of the universe and/or the social sciences.

To account for this ecosystemic complexity, to understand the resilience of the ecological processes and to open the possibility of ecosystem management and control, require to articulate various strategies: for reconstructing the spatial and temporal dynamics, starting from observations and from increasingly instrumented experiments; for theoretically and experimentally identifying the retroactive mechanisms and the emergence phenomena; for modeling and validating these models.

### **Grand challenges:**

1. Develop observation and experimental systems for the reconstruction of the long-term dynamics of ecosystems.
2. Model the relationships between biodiversity, functioning and dynamics of the ecosystems.
3. Associate integrative biology and ecology to decipher evolutionary mechanisms.
4. Simulate virtual landscapes (integration and coupling of biogeochemical and ecological models into dynamic landscape mock-ups).

### **1. Develop observation and experimental systems for the reconstruction of the long-term dynamics of ecosystems.**

Improvement of in situ systems of measurement (metrology and sensors); integration of data resulting from networks of observation (spatial and temporal sampling strategies, environmental research observatories) and/or of experiments (microcosms, mesocosms) in models of ecosystems; development of information systems based on a conceptual modeling of the studied ecosystems; multidimensional analysis of data coming from multiple sources (“meta-analysis”?); search of invariants or adimensional parameters which enable upscaling.

## **2. Model the relationships between biodiversity, functioning and dynamics of the ecosystems**

These relations, which play a central part in the very vast field of the studies relating to the biodiversity, are declined for various functions (production, transfers of matter and energy, resistance and resilience to perturbations, etc.), at different scales of space (station, landscape, area, continent) and of time, with the difficulty in articulating the short time of “functioning”? and the long time of the “dynamics of the structures”? Historically, the study of these relations was approached according to two reciprocal points of view: initially, wondering about the way the environment and the functioning of the living organisms and their interactions determine the assemblies of species; more recently, and in a reciprocal way, by studying the role of the richness and specific diversity in the way ecosystems function.

## **3. Associate integrative biology and ecology to decipher evolutionary mechanisms**

To understand and model the response of the communities (structure, functioning and dynamics) to the changes of their environment (climatic changes, pollution, biological invasions, etc.) rest mainly on a better comprehension of the adaptive mechanisms. This task can now be supported by conceptual, methodological and technological progress made in integrative biology (genomic functional calculus, biology molecular, genetic, physiology and ecophysiology) and by the convergence of approaches from population, molecular and quantitative genetics.

## **4. Simulate virtual landscapes (integration and coupling of biogeochemical and ecological models into dynamic landscape mock-ups)**

Conception of virtual mock-ups, based on a categorical representation of the landscape mosaic, would make it possible to build a typology of representative landscapes (hedged farmland, open field, mixed landscapes, forests, peri-urban areas, etc...). The following phases would consist in modeling: on the one hand, the functioning of the landscape (i.e. biogeochemical cycles, transfers and exchanges: air particulate transport, determinism of the microclimate, transport of water and of associated pollutants in the soil and the watersheds) with as a deliverable the production of functional relations between landscape topology and structure of the exchanges; on the other hand, the very dynamics of the landscape (i.e. evolution of its space organization) under the effect of the human activities and of certain ecological processes (for example, colonization of spaces by the vegetation). Such a tool would have a great utility in ecology or epidemiology, in the agronomic disciplines and for the local management of the territory.

## **5. Design decision-support systems for multifunctional ecosystems**

Qualification and quantification of the products and services provided by the ecosystems; integration of these services and products in systems of indicators (dashboards, tools of decision-making assistance, life cycle analysis and eco-balance analysis, etc.); formalization and quantification of the perturbation regimes, the human practices and techniques, or the management systems relating to the ecosystems; coupling of models of different nature; taking into account of the stochastic components (whether those are intrinsic or that they are related to the incomplete character of knowledge on the elements of these systems, their interactions and the extrinsic factors likely to disturb them); multifactorial optimization.

## 2.5. From individual cognition to social cognition

**Reporter:** David Chavalarias

**Contributor:** Paul Bourguine, David Chavalarias, Jean-Philippe Cointet, Guillaume Deffuant, Camille Roth.

**Keywords:** Social dynamics, decision criteria modeling, quantitative social measurement, social cognition, inter-individual heterogeneity

Cognition is information processing, understood in a wide sense, that is, including all related aspects such as, for instance, interpretation processes. A cognitive system is thus an information processing system. It can be embedded in a single individual or distributed over a large number of individuals. We would talk of individual cognition or distributed cognition. Social cognition is a cognitive process distributed over all members of a society, interacting within a social network. Individual cognition as well might be considered as distributed cognition over a neural network.

In social networks, some information reaches some agents, then its content is processed by the social network, producing other pieces of information and other social links following series of interactions. This process of social cognition could thus lead to a transformation of the social network.

At individual and collective levels alike, cognitive processes are obeying strong constraints: individuals cannot achieve anything outside of what they are able to do themselves or in interaction with others; nothing can be anticipated outside of what they can predict alone or by interacting with others. Both the network structure and the nature of interactions are as such strong constraints on cognitive processes.

New protocols appear which make it possible to describe or quantify these constraints at the infra-individual, individual and collective levels, thus suggesting, in turn, new models. The quick migration of social interactions towards digital media enables the massive collection of data on social cognition, from the viewpoint of both its processes (spatial structure of interactions, temporal distributions, etc.) and its products (online documents, user-focused data, etc.). The coexistence of these two phenomena opens today new perspectives for the study of individual and social cognition on the basis of benchmarking models with empirical data. This ought to be a major ambition for a better understanding of the evolution of our societies.

### Challenges

- 1st Challenge: Individual cognition, cognitive constraints and decision processes
- 2nd Challenge: Modeling the dynamics of scientific communities
- 3rd Challenge: Society of the Internet, Internet of the society

### 1st challenge: Individual cognition, cognitive constraints and decision processes

The relationship between high-level and low-level cognitive processes remains an unsettled issue: the link between dynamic processes in the neural network and symbolic processes as they are being studied by psychology and linguistics is still open to question. A promising

approach consists in exploring in a much more precise manner meso-scale spatio-temporal dynamics, like for example cortical columns, synchronized neural assemblies (or, more broadly, polysynchronous assemblies). These spatio-temporal dynamics may be useful in attesting symbolic processes. In order to understand better the transition from dynamic and symbolic processes, a theoretical and methodological questioning, as well as sharing data from very large databases provided with their metadata appears to be unavoidable.

Significant progress towards this challenge would not only lead to unifying an essential aspect of cognitive science, but would also launch much more strongly the new discipline of neuroeconomics: observing neural activity brings a novel viewpoint on the study of human behavior towards « nature » or in relation with strategic and social interactions with other individuals. From the perspective of cognitive economics, this brings hopes that decision theory could be revisited, as well as standard game theory, including the notions of « preference » and « utility » which are funding economic theory.

## **2nd challenge: Modeling the dynamics of scientific communities**

Scientific communities constitute a privileged area for the study of social cognition because both the structure of the underlying networks (team organization, collaboration networks, co-authorship networks, citation networks) and the production of these communities (conferences, journals, papers) is known in a dynamic fashion. In order to exchange concepts, scientific communities create their own language whose evolution reflects their own activity. This makes it possible to address very precise topics pertaining to how these scientific communities are collectively processing information – to cite a few: how new concepts or new issues are being adopted? What are remarkable structures for innovation diffusion (effect of authorities, local traditions, etc.). What is the effect of the breakdown of individuals in communities or the creation of links between communities on the development of knowledge? Which are the relationships between individual trajectories and community evolutions? What tools should we create to visualize dynamically the evolution of scientific paradigms, taking into account the continuing input of scientific production?

**Keywords:** scientometrics, epistemology, collective discovery, concept diffusion, collaboration networks.

Examples:

- Emergence and diffusion of new concepts in bibliographical databases
- Detection of emerging scientific fields
- Dynamics of collaboration networks
- Paradigmatic comparison of distinct scientific communities or institutions

## **3rd challenge: Society of the Internet, Internet of the society**

The quantity of information stored on the Internet will soon have strongly overwhelmed that stored on paper. The Internet concentrates today various types of knowledge storage systems (papers, encyclopedias, etc.). It is also a place where discussions (weblogs, forums) and commercial transactions (auction and trade websites) occur, referencing is being produced (for individuals through personal webpages as well as for institutions and organizations), it is place which serves as an external memory for relationship networks (friendship networks, workgroups, etc.) and, also, it is a « world agenda » with hundreds of thousands of events

which are being announced every day. What modifications this new tool is presently bringing to social cognition processes (new kinds of encounters, new kinds of exchange, new kinds of debates, new kinds of collective building of knowledge)? For the first time, we may empirically work on this type of data with a fairly large spatio-temporal precision. How could we use these new sources of information to better understand social dynamics and create and provide tools to visualize the complexity of social activity which the Internet is revealing? A major challenge is to transform raw information available from the Internet in structured flows of information which make it possible to visualize, model and rebuild social cognition processes at work on the web, in a multiscale fashion.

**Keywords:** Geolocalized indexing, social emotion diffusion, epistemic communities, social dynamics and cultural evolution, visualization, collective building of knowledge.

**Examples:**

- Impact of weblogs in political and civil debates,
- New dynamics for the collective elaboration of knowledge (Wikipedia, open-source software, etc.) ,
- Measuring the propagation of social emotion following important social events, through the number of requests (ex: Google trends) ,
- Comparative study of cultural differences through geo-localized informations (semantics in webpages, tags, requests on search engines, etc.), reconstruction of cultural territories.
- Formation of epistemic communities, friendship networks

## 2.6. Innovation, learning and co-evolution

**Reporter:** Denise Pumain

**Contributor:** David Chavalarias, Nadine Peyrieras, Denise Pumain

### **Innovation, learning and co-evolution**

Novelty in complex systems appears under a variety of processes, through the emergence of new entities and new categories, through the modification of interaction processes, through changes of their temporal or spatial scales, through their dynamical transformation. Within a complex system science perspective, the main question is to know whether the modes of change are comparable when going from natural and artificial towards social systems. A first challenge is to identify which dynamic conditions are favorable to innovation. Is innovation always associated to jumps, ruptures or bifurcations, or can it proceed from more regular trends? Which processes are explaining the frequent observation of innovation cycles? A second challenge is to determine whether there is an acceleration of innovation in human society through time, by identifying relevant measures of societal changes. A third challenge is to understand how intention and reflection are framing the innovation in social systems and how the feedback effect of learning affects individual and collective cognition over historical time.

**Keywords:** innovation, emergence, bifurcation, co-evolution, learning, acceptance, society of information

### **Grand challenges:**

1. Understanding dynamic conditions of innovation
2. Modeling innovations and their rhythms
3. Understanding the relation between cognition and innovation

### **1. Understanding the dynamic conditions of innovation**

Can innovation only be analyzed ex-post, or can it be predicted, from which indicators and explanatory variables? Are the signs that announce the change in a specific regime of the system's dynamics, through the amplification of fluctuations around a trajectory, through intensification of pre-existing processes, or through the transition between quantitative toward qualitative variations? How innovation becomes accepted, through introducing itself in existing structures or by replacing them, or by inducing modifications of these structures, which make them compatible? Which relationships are established between new artefacts, new functionalities and the new practices that use them? What kind of factors the learning processes have to combine in order to link these different aspects together? How can be explained the formation of subsets of many innovations which lead to the observation of large cycles in the evolution?

### **2. Modeling innovations and their rhythms**

Certain analysts suggest that there is an acceleration of the production frequency of innovations, especially through the technical revolutions and the evolution towards a society of information. Is this observation a reality or an illusion? Answering that question requires a

rigorous definition of innovation and of information and careful determination of the time intervals that measure its frequency. How to build reference times that are relevant for characterizing the rhythms of emergence, succession and co-presence of innovations? In other words, is the regular hour time meaningful or should one imagine other measures of societal time?

### **3. Understanding the relation between cognition and innovation**

Societies build and assimilate innovations that concern as well the artefacts that they produce as their own practices and the institutions they create. Is it possible to understand the social dynamics of innovation without introducing the individual and collective intentionality and reflexivity? Is social innovation in continuity or in rupture with biological evolution? Does the fact that innovation is targeted, that the selection of innovation is guided, that the processes of learning and acceptance are conveyed through legal, economic or cultural regulations introduce different characteristics and effects for innovation in human societies? Within these processes, is it possible to identify at meso-levels social milieux or networks or geographical spaces that would be more favorable to innovation, or loaded with a specific innovative capacity? What are the expressions of the interactions between innovation and individual cognition? Can the social control on innovation reach as far as the biological transformations?

## 2.7. Territorial intelligence and sustainable development

**Reporter:** Denise Pumain

**Contributors:** Pierre Auger, Olivier Barreateau, Jean-Bernard Baillon, Rémy Bouche, Danièle Bourcier, Paul Bourguine, Elisabeth Dubois-Violette, Jean-Pierre Gaudin, Elisabeth Giacobino, Bernard Hubert, Jean-Pierre Leca, Jean-Pierre Muller, Ioan Negrutiu, Denise Pumain.

### **Territorial intelligence and sustainable development**

A physical territory is a system that naturally integrates a variety of processes usually analyzed by a diversity of disciplines (economics, sociology, and so on). These processes activate natural and social resources and include individual and collective strategies, whose dynamics are coupled in building the territory. Planned and unplanned actions as well as reiterated practices and strategic anticipations are taken by households, firms or government bodies. Physical infrastructures as well as immaterial long lasting socio-spatial configurations constrain these actions and also shape the territory at several scales in space and time. For mastering that complexity, simulation models are needed: for understanding the relationship between processes and structures; for evaluating and preparing individual and collective action; for measuring their impact on the viability of spatial structures. Such models are important issues for helping decision-making and may then contribute to change the evolution of territories.

**Keywords:** geographical space, territorial configuration, rural and urban regions, networks, systems of cities, multi-level and multi-actor governance, resources, regulation, sustainable development, negotiation, geographical information systems, cellular automata, spatial simulation, multi-agents systems;

### **Grand challenges:**

1. Understanding territorial differentiation.
2. Towards a reflexive territorial governance
3. Viability and observation of territories

### **1 Understanding territorial differentiation**

Territories are reorganized at different scales, from local to global, through the expansion of material and immaterial networks and the diversification of levels where decision take place. “Network territories”? are forming by articulating places according to connectivity and not only in continuity, at the level of individuals as well as at the level of global firms. In parallel contiguous territories are partially intersecting, for instance when their future is governed by several decision centers. Are the classical territorial models still valid for representing geographical differences? How can they be replaced?

The evolution of territories is usually described in terms of geohistory, territorial viability, or adaptation and innovation capacity. It must be related to processes as institutions, technological innovations, transformations of social practices and representations. Within that dynamics, modes of circulation and concentration of information are essential. Very often, the networks that convey information are not observable; they have to be reconstructed through

simulation models. The challenge is to couple dynamic models representing spatial interactions at a variety of scales and geographical information systems that can integrate and visualize the located information and the evolution of networks and territories.

## **2 Towards a reflexive territorial governance**

Territorial governance is no longer a simple hierarchical top down control but a multi-level and multi-actor process. Intermediate control structures are emerging between territorial scales. New models of legitimating are invented between representative and participative democracy and inclusive governance. Moreover, the growing interest for sustainability invites to take into account the natural dynamics that operate at different scales of time and space as well.

The building of a well-informed, “reflexive”? governance, relies on the invention of new decision models which consider processes and institutions, configuration of competition and cooperation, symbolic and practical interactions. Natural and social dynamics have to be coupled in identifying organization levels, scales of time and relevant territorial subdivisions for a reflexive control. A further difficulty is to include the diversity of the strategies of the actors in such models. Generally speaking, the question is to identify which structures are emerging at meso level and to understand what are the linkages between micro, macro and meso levels.

## **3 Viability and observation of territories**

The retrospective and prospective analysis of territories is essential for improving knowledge about the long- term sustainability of geographical entities in their social, economic, ecologic and ethic dimensions. Questions of measurement are fundamental. Choosing indicators, their weighting, defining norms, identifying objectives and stakes are specific problems for territories that are both complementary and competitive. More reliable spatio-temporal databases are needed for measuring the evolutions and comparing territorial dynamics.

The challenge is to organize the comparability of territorial dynamics. A major issue is to adapt or create sources of information that were established for administrative or political units at a given period in time, for evaluating territorial entities (cities, regions, networks) that have their own dynamics. The problem is crucial for long-term studies of the resilience and vulnerability of urban systems, or for a comparative evaluation of agenda 21 programs (which combine societal, economic and ecological objectives).

## 2.8. Ubiquitous computing

**Reporter:** Marc Schoenauer

### Ubiquitous Computing

Today's technology makes it possible and even necessary to radically change the way we gather and process information, from the monolithic approach to the networked collaboration of a huge number of possibly heterogeneous computing units.

This new approach should be based on distributed processing and storage, and will allow us to add intelligence to the different artefacts that are more and more present around us, and to compensate the foreseeable limits of classical Computer Science (end of the Moore era). This long term objective requires

- solving issues related to physical layout and communications (distributed routing and control)
- setting up self-regulating and self-managing processes
- designing new computing models
- specifying adaptive programming environments (using Machine Learning, retro-action and common sense).

### Challenges

- Local design for global properties (routing, control, confidentiality)
- Autonomic Computing (robustness, redundancy, fault tolerance)
- New computational models: distributing processing and storage, fusion of spatial, temporal and/or multi-modal data, abstraction emergence
- New programming paradigms: creation and grounding of symbols (including proof and validation)

### Keywords

- Peer to Peer networks (P2P)
- Ad hoc networks
- Observation of multiscale spatio-temporal phenomena (trophic networks, agriculture, meteorology, ...)
- Epidemic Algorithms
- Computational Models and Information Theory
- Spatial computing
- Self-aware systems
- Common Sense
- Privacy

### Preamble

It seems clear that we have today reached the technological limits of Von Neumann's sequential computational model. Hence new paradigms are necessary to fulfill the ever-growing demand for computational power of our modern society. The heart of those new paradigms is the distribution of computing tasks on decentralized architectures (e.g. multi-core processors and computer grids). The complexity of such systems is the price to pay to

address the scaling and robustness issues of decentralized computing. Furthermore, it is now technologically possible to flood the environment with sensors and computing units wherever they are needed. However, an efficient use of widely distributed units can only be achieved through networking — and physical constraints limit the communication range of each unit to a few of its neighbors (ad hoc networks). At another scale, the concept of P2P networks also implies a limited visibility of the whole network. In both cases (ad hoc and P2P networks), the issue is to make an optimal use of the complete data that is available on the whole network. The challenges in this framework are targeted toward the new computational systems, but will also address some issues raised in social or environmental networks, that are treated in other pages of this road-map.

## **Local design for global properties**

### *Routing, control and privacy*

In order to better design and maintain large networks, we need to understand how global behaviors can emerge even though each element only has a very limited vision of the whole system, and makes decisions based on local information. A base model is that of epidemic algorithms, in which each element exchanges information with its neighbors only. The important issues are the type of informations that are exchanged (that should take into account privacy constraints) and the selection of corresponding neighbors. Both choices influence the global behavior of the system.

**Methods:** Information theory; dynamical systems; statistical physics; epidemic algorithms; bio-inspired algorithms

## **Autonomic Computing**

### *Robustness, redundancy, fault tolerance*

Large scale deployment of computational systems will not be possible without making those system autonomous, in a way that resemble properties of living systems: robustness, reliability, resilience, homeostasis. However, the size and heterogeneity of such systems make it difficult to come up with analytical models; moreover, the global behavior of the system also depends on the dynamical and adaptive behavior of the whole set of users.

**Methods:** Bio-inspired systems, self-aware systems.

## **New computing paradigms**

### *Distributed processing and storage, fusion of spatial, temporal and/or multi-modal data, abstraction emergence*

The networking of a large number of possibly heterogeneous computational units (grids, P2P, n-core processors) gathers a huge computational power. However, in order to efficiently use such power, new computing paradigms must be designed, that take into account the distribution of information processing on weak or slow units, and the low reliability of those units and of the communication channels. Similarly, data distribution (sensor networks, RFID, P2P) raises specific challenges: integration, fusion, spatio-temporal reconstruction, validation.

**Methods:** Neuro-mimetic algorithms, belief propagation.

### **Specification of adaptive programming environments**

*machine learning, retro-action and common sense*

Programming ambient intelligence systems (domotic, aging, fitness) must include the user in the loop. The specification of the expected user behavior requires a transparent link between the low level data that are available and the user's natural concepts (e.g. symbol grounding). On the other hand, the research agenda must start by studying actual habits; such co-evolution of the user and the system leads to hybrid complex systems.

**Methods:** Brain Computer Interface, programming by demonstration, statistical learning.

## 2.9. Geosciences and the environment

**Reporter:** Michael Ghil

**Contributors:** Pierre Baudot, François Daviaud, Bérengère Dubrulle, Patrick Flandrin, Cedric Gauchere, Gabriel Lang, Francesco d'Ovidio, Daniel Schertzer, Eric Simonet.

**Keywords:** Climate change, predictability and uncertainties, ecosystems and landscapes, multiple scales and heterogeneity, climate and trophic networks, emergent diseases, transport and mixing, climate -weather interactions, stochastic vs. deterministic modeling.

### Introduction

The physical, chemical and biological environment of humans – from the local, community level to the global, planetary one – represents a rapidly increasing concern of the post-industrial era. Its study involves all the subsystems of the Earth system – the atmosphere, oceans, hydro- and cryosphere, as well as the solid Earth's upper crust – along with their interactions with the biosphere and with human activities. We are therefore dealing with a highly complex, heterogeneous and multiscale system, and with an exceedingly interdisciplinary set of approaches to it. The concepts and tools of complex-system theory seem particularly useful in attacking three major challenges. Firstly, the range of uncertainties still prevailing in future climate change projections has until now been attributed largely to difficulties in parameterizing subgrid-scale processes in general circulation models (GCMs) and in tuning semi-empirical parameters. Recent studies also point to fundamental difficulties associated with the structural instability of climate models and suggest applying the theory of random dynamical systems to help reduce the uncertainties. Secondly, the Earth system varies at all space and time scales and is thus out of and probably far from thermodynamic equilibrium. The methods of statistical physics are therefore of interest in modeling the system's near-equilibrium behavior and then extending the results farther away from equilibrium. Finally, much of the interest in this area arises from concern about the socio-economic impact of extreme events. The study of their statistics and dynamics can lead to a deeper understanding and more reliable prediction of these events.

The physical, chemical and biological environment of humans – from the local, community level to the global, planetary one – represents a rapidly increasing concern of the post-industrial era. The system's complexity is certainly comparable to that of systems studied in the life or cognitive sciences. It therefore appears highly appropriate to include this major area of applications of complex-system theory into the concerns of this road map.

The Earth system involves several subsystems – the atmosphere, oceans, hydro- and cryosphere, as well as the solid Earth's upper crust – each of which in turn is highly heterogeneous and variable on all space and time scales. Moreover, this variability is affected by and in turn affects the ecosystems hosted by each subsystem, as well as humans, their economy, society and politics. We are thus dealing with a highly complex, heterogeneous and multiscale system, and so the scientific disciplines needed to better understand, monitor, predict and manage this system are diverse and numerous. They include various subsets of the physical and life sciences, mathematics and informatics, and of course the full set of the geo- and environmental sciences, from geology, geophysics and geochemistry to the atmospheric and oceanic sciences, hydrology, glaciology and soil science.

Among the key interdisciplinary issues that arise in this major area are future climate change, change in the distribution of and interaction between species given past, present and future climate change, the way that the biogeochemical cycles of trace chemicals and

nutrients interact with other changes in the system, and the connection between health issues and environmental change. On the methodological side, major objectives that would help to solve these issues include better prediction and reduction of uncertainties, better description and modeling of the transport and mixing of planetary fluids, understanding the net effect of weather on climate and the changes in weather as climate changes. Understanding the best uses of stochastic, deterministic or combined modeling in this highly complex setting is also essential.

To deal at the same time with some of these key issues and attempt to achieve some of the associated major objectives, we propose to focus on the following three main challenges: (i) to understand the reasons for and reduce the uncertainties in future climate change projections; (ii) to study the out-of-equilibrium statistical physics of the Earth system, across all scales; and (iii) to investigate the statistics and dynamics of extreme events.

The range of uncertainties in future climate change projections was originally determined in 1979 as an equilibrium response in global temperatures of 1.5–4.5 K for a doubling of atmospheric CO<sub>2</sub> concentration.

After four IPCC assessment reports, it is still of a few degrees of end-of-century temperatures for any given greenhouse gas scenario. This persistent difficulty in reducing uncertainties has, until recently, been attributed largely to difficulties in parameterizing subgrid-scale processes in general circulation models (GCMs) and in tuning their semi-empirical parameters. But recent studies also point to fundamental difficulties associated with the structural instability of climate models and suggest applying the theory of random dynamical systems to help reduce the uncertainties.

The Earth system varies at all space and time scales, from the microphysics of clouds to the general circulation of the atmosphere and oceans, from micro-organisms to planetary ecosystems, and from the decadal fluctuations of the magnetic field to continental drift. The entire system, as well as each of its subsystems, is a forced and dissipative system and is thus out of thermodynamic equilibrium and probably far away from it. The methods of statistical physics therefore seem of interest in modeling the system's near-equilibrium behavior and trying to derive results that might then be extended to more realistic settings, farther away from equilibrium.

Finally, much of the interest in the geosciences and the environment arises from concern about the socio-economic impact of extreme events. The standard approach to such events rests on generalized extreme value theory (GEV). Its assumptions, however, are rarely met in practice. It is therefore necessary to pursue more sophisticated statistical models and to try to ground them in a better understanding of the dynamics that gives rise to extreme events. Based on better statistical and dynamical models, we should be able to provide more reliable predictive schemes for extreme events, and subject them to extensive testing across disciplines and data sets.

The geosciences have a long tradition of contributing to the study of nonlinear and complex systems. The work of E.N. Lorenz in the early 1960s has provided a major paradigm of sensitive dependence on initial state. His work and that of C. E. Leith have yielded deep insights into error propagation across scales of motion. Multiscale phenomena in the solid-earth and fluid-envelope context have helped refine the understanding of multi-fractality and its consequences for prediction across disciplines, even in the social and political sphere. We hope and trust that the work proposed here will prove equally inspiring and fruitful for the theory of complex systems and its applications in many other disciplines.

## New challenges

### 1. Understanding and reducing uncertainties.

Charney et al. (Natural Academic Press, 1979) were the first to attempt a consensus estimate of the equilibrium sensitivity of climate change in atmospheric CO<sub>2</sub> concentrations. The result was the now famous range of 1.5K to 4.5K of an increase in global near-surface air temperatures  $T_s$  given a doubling of CO<sub>2</sub> concentrations. Earth's climate, however, never was and probably never will be in equilibrium. In addition to estimates of equilibrium sensitivity, the four successive reports of the Intergovernmental Panel on Climate Change (IPCC: 1991, 1996, 2001, 2007) therefore focused on estimates of climate change over the 21st century, based on several scenarios of CO<sub>2</sub> increase over this time interval. The general circulation models (GCM) results of temperature increase over the coming 100 years have stubbornly resisted any narrowing of the range of estimates, with results for end-of-century  $T_s$  still ranging over several degrees Celsius, for a fixed CO<sub>2</sub> increase scenario. This difficulty in narrowing the range of estimates is clearly connected to the complexity of the climate system, the nonlinearity of the processes involved and the obstacles to a faithful representation of these processes and feedbacks in GCMs.

One obvious source of errors is the difficulty of representing all the processes that fall below the spatial and temporal resolution of the model. This problem is especially evident for biochemical processes, where the microphysical and microbiological dynamics is coupled to the turbulent dynamics of the ocean and atmosphere and produces a spatiotemporal variability at virtually any scale of observation. One example is phytoplankton, whose fundamental role in absorbing CO<sub>2</sub> is affected as much by the nutrient advection due to the large-scale circulation (basin scale, years), as by the presence of upwelling filaments (1-20 km, days), the ecological interaction with zooplankton (mm/m, hours/days), or the turbulent and biological processes at the cell scale. The study of such biochemical phenomena requires the development of novel theoretical tools that are beyond the capability of individual disciplines but which, because of their characteristics, fall naturally into the framework of complex systems. Such studies should be able to:

1. deal at the same time with the various spatial and temporal scales of transport and tracer dynamics;
2. integrate descriptions of different disciplines, notably transport and mixing properties from turbulence theory, and the biological and/or chemical processes of the advected tracer;
3. provide results in a form that can be compared with ever-expanding observational datasets;
4. and finally, allow to formulate a computationally-efficient parameterization scheme for circulation models.

A second source of errors lies in the fundamental difficulty related to the structural instability of climate models. It is well-known that the space of all deterministic, differentiable dynamical systems (DDS) has a highly intricate structure: the structural stable systems are unfortunately not typical of all deterministic dynamics, as originally hoped (Smale, 1967). Indeed, what is modeled by DDS does not appear to be typically robust from a qualitative, topological point of view, even for small systems like the Lorenz (1963) model. This disappointing fact has led mathematicians to grasp the problem of robustness and genericity with the help of new stochastic approaches (Palis, 2005). On the other hand, work on developing and using GCMs over several decades has amply demonstrated that any addition or change in a model's "parameterizations" - i.e. in the representation of subgrid-scale

processes in terms of the model's explicit, large-scale variables - may result in noticeable changes in the model solution's behavior.

The range of uncertainties issue, far from being a mere practical difficulty in "tuning" several model parameters, could be related to the inherent structural instability of climate models. A possible way of reducing this structural instability is the use of stochastic parametrizations with the aim of smoothing the resulting dynamics through ensemble average. A key question is then to determine whether ad-hoc stochastic parametrizations add some form of robustness to known deterministic climate models, and how they can reduce the range of uncertainties in future climate projections. Preliminary results indicate that noise has stabilizing effects that need to be investigated across a hierarchy of climate models from the simple to the most complex GCMs. Such an idea could be tested using theoretical concepts and numerical tools from the theory of random dynamical systems (RDS; L. Arnold, 1998). In this purely geometrical theory, noise is parametrized so as to treat stochastic processes as genuine flows living in an extended phase space called a "probability bundle". Random invariant sets such as random attractors can then be defined and rigorously compared, using the RDS concept of stochastic equivalence, thereby enabling us to consider the structural stochastic stability of these models.

## **2. Out-of-equilibrium statistical physics of the Earth system**

The Earth and its various components (hydrosphere, atmosphere, biosphere, lithosphere) are typical out-of-equilibrium systems: due to the intrinsic dissipative nature of their processes, without forcing they are bound to decay to rest. However, in the presence of permanent forcing, a steady state regime can be established, in which forcing and dissipation equilibrate on average, allowing the maintenance of non-trivial steady states, with large fluctuations covering a wide range of scales. The number of degrees of freedom involved in the corresponding dynamics is so large that a statistical mechanics approach - allowing the emergence of global relevant quantities to describe the systems - would be welcome. Such a simplification would be especially welcome in the modeling of the fluid envelopes, where the capacity of present computers prohibits the full-scale numerical simulation of the (Navier-Stokes) equations describing them. Similar problems are ubiquitous in biology and environment, when the equations are known.

Another interesting outcome of a statistical approach would be to derive an equivalent of the Fluctuation-Dissipation Theorem (FDT), to offer a direct relation between the fluctuations and the response of the system to infinitesimal external forcing. Applied to the Earth system, such an approach could provide new estimates of the impact of climate perturbation through greenhouse gas emissions.

Various difficulties are associated with the definition of out-of-equilibrium statistical mechanics in the earth system, including:

- the problem of the definition of an entropy (possibly an infinite hierarchy of them) in heterogeneous systems;
- the identification of the constraints;
- the problem of the non-extensivity of the statistical variables, due to correlations between the different components of the system (possibly solved by introducing effective (fractional) dimensions).

On the physical side, several advances have been made recently in the description of turbulence, using tools borrowed from statistical mechanics for flows with symmetries. Variational principles of entropy production are also worth considering. Other advances have been made with regard to the equivalent of the FDT for physical systems far from equilibrium. Experimental tests in a glassy magnetic system have evidenced violation of the

FDT through non-linearities in the relation between fluctuation and response. General identities between fluctuation and dissipation have been theoretically derived only for time-symmetric systems. They have been experimentally tested successfully in dissipative (non time-symmetric) systems like electrical circuits or turbulent flow. It would be interesting to extend these results to the Earth system.