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# TACKLING COMPLEXITY IN SCIENCE

General Integration of the Application of Complexity in Science

PROJECT REPORT

A NEST PATHFINDER INITIATIVE

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# Tackling Complexity in Science

## General Integration of the **A**pplication of **C**omplexity in **S**cience

edited by  
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and  
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There is no commonly accepted definition of "*complexity*". Nevertheless, it is clear that widely differing systems, composed of many interacting units, generate under certain conditions a characteristic common phenomenology, the most prominent signature of which is the "emergence" of new patterns transcending the characteristics of the individual units.

The promise of the *science of complexity* is to provide, if not a completely unified approach, at least *common tools* to tackling complex problems arising in a wide range of scientific domains.

NEST, *New and Emerging Science and Technology*, is initiative under the European Commission's Framework Programme 6 to promote highly interdisciplinary, high-risk research. NEST launched a number of focussed "PATHFINDER" initiatives, including "*Tackling Complexity in Science*".

The "*Tackling Complexity*" initiative aims at encouraging the development and transfer from one area of science to another of solutions and approaches to concrete complex real-world problems. Such solutions need, at the same time, to hold the promise of being more generalisable.

The initiative undertook two calls for proposals (2004 and 2006) which resulted in the funding of 23 STREP *focussed* research projects and one Coordination Action, GIACS, amounting to approximately 35 M Euro worth of new research funding.

The goal of GIACS (*General Integration of the Application of Complexity in Science*) is to serve as a forum to bring the research of these research projects together and help in their relationship with the ongoing research in the field of Complexity in Europe and the rest of world.

The current report is one of the deliverables of GIACS and serves to speculate about the future directions and opportunities of complexity research in the long term. It is the result of the interaction of large number of outstanding scientists involved in GIACS and other NEST-Complexity projects. It is intended to be speculative and thought provoking, while at the same time serving as an inspiration for future research directions in the field.

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## EXECUTIVE REPORT

A theory of complex systems has been developed from the forties, relating simple elementary processes to collective functional properties in physics, biology and the social sciences.

More recently, applications to design and business have been developed.

A major turning point around the year 2000 is the availability of huge sets of data which complex systems methodology allows to transform into useful knowledge.

A list of promising research avenues would include:

- From model systems to real world systems.
- Inverse dynamics especially in biological networks, but also in many other fields such as markets or crowds when data become available.
- Distributed processing in the industry and services, starting with the Internet, data processing, etc. find solution which are distributed, scalable and adaptive.
- A nearly unchecked field is policy design: defining a policy and checking its consequences by what/if simulations; policy implementation taking into account the adaptivity of both measures and constituency.

Among the general issues are:

- Since complex systems is such an invasive methodology applicable to so many fundamental and applied fields of research, a preliminary question is: does it make sense to have specific calls about complex systems research or should we rather keep the standard calls specific of the domain of application? In the long run one can hope for a better integration of field research and complex systems specialists which would allow mixed collaborations to answer domain specific calls. Presently, this integration is far from achieved; it would thus be appropriate to maintain some calls inside a STREP Pathfinder complexity initiative as was previously done with such programs as *what it means to be human*, *tackling complexity in science*, *synthetic biology*, etc.
- Education. Promote education in complex systems methods and results both at intermediate (master and doctorate) and elementary level. Most of this effort (writing books, manuals, paper series, or equivalent web sites, syllabus design, summer schools, libraries, etc.) has to be done by the scientific community. But the European Commission (EC) could consider supporting coordination actions built to promote education. At the master or even undergraduate level, it is important to ensure that specialists in biology or social science understand the reach of complex systems methods. The EC might also support some effort to translate documents. Such an effort could help for instance students from Eastern countries to readily access this literature, but could also help the diffusion of good material produced in Eastern Europe.
- Databases. Sustain efforts to maintain large and easily accessible data bases. The situation is very contrasted between different fields. Public databases are available in genomics. The same is true for many financial time series. This is not the case for social sciences. In economics, many valuable data about individual firms such as production, trading links, employment patterns are confidential in Europe. Even data collected thanks to the European Commission financial support are not generally available. Making such data generally available would have a strong positive impact on sound-based research and would of course finally benefit the industry and government. Unfortunately, solutions are not obvious.



# 1 INTRODUCTION

## ***1.1 From components to global properties***

The challenge

Let us exemplify the challenge of complex system research with the mind/brain issue. The brain is composed of  $10^{11}$  interacting neurons which can be considered as electric cables (axons) with chemical connexions (synapses). How can we deduce the mind properties (cognition) from the brain structure? More generally, how can we explain the functional organization of biological systems at the level of organs for instance, from the properties of their components (from neurons to mind or from lymphocytes to the immune response)?

Similar questions arise in the social sciences; can we understand social organizations (institutions) and collective behaviour from the properties of the human agents which compose them? Such a research program is called methodological individualism in the social sciences.

Can we define complex systems?

The answer is yes, but some caution should be used in keeping in mind the difference between real world complex systems and their models.

Let us start with models: complex systems are composed of a very large number of different elements with non-linear interactions; furthermore the interaction structure, a network, comprises many entangled loops.

The purpose of complex system research is to propose and solve models such that we can deduce the functional organization from the interaction of the components. But to handle such large systems, the description of their elementary components is generally oversimplified with respect to real systems: hence the issue of the comparison between the predictions of the model with the real system. We will see that complex system theory often addressed the issue by restricting predictions to generic properties. (A recent shift in interests occurred with the availability of large data sets in biology or social sciences).

Before addressing the issue of generic properties, which can be rather technical, let us discuss one of the caricatures of complex systems: complex systems is a theory of the whole, in other words it is so general that it has no practical use. Let us use at this stage some comparisons.

Thermodynamics is not only a theory about work and heat but it applies to all physical systems: gases, liquids, solids with electric, magnetic or elastic properties. In fact statistical mechanics, the microscopic theory behind thermodynamics, is probably the closest theoretical analogue to complex systems theory: its purpose is to deduce the macroscopic properties of matter from those of its individual components, atoms, molecules, polymers. But not all properties of matter rest on thermodynamics: optical properties can often be deduced by adding up properties of individual atoms. The fact that some answers can be obtained from complex systems theory, does not mean that complex systems theory exhausts all fields of research. There are many other approaches of real systems with little direct connection with complex systems methodology: experiments, empirical data collection, monographs, etc. Even if we consider complex systems theory as particularly well adapted to the formalization of problems in biological and social sciences, it does not imply that it should be the only approach to logical or mathematical formulations.

The projection perspective is probably an appropriate metaphor (see figure 1).

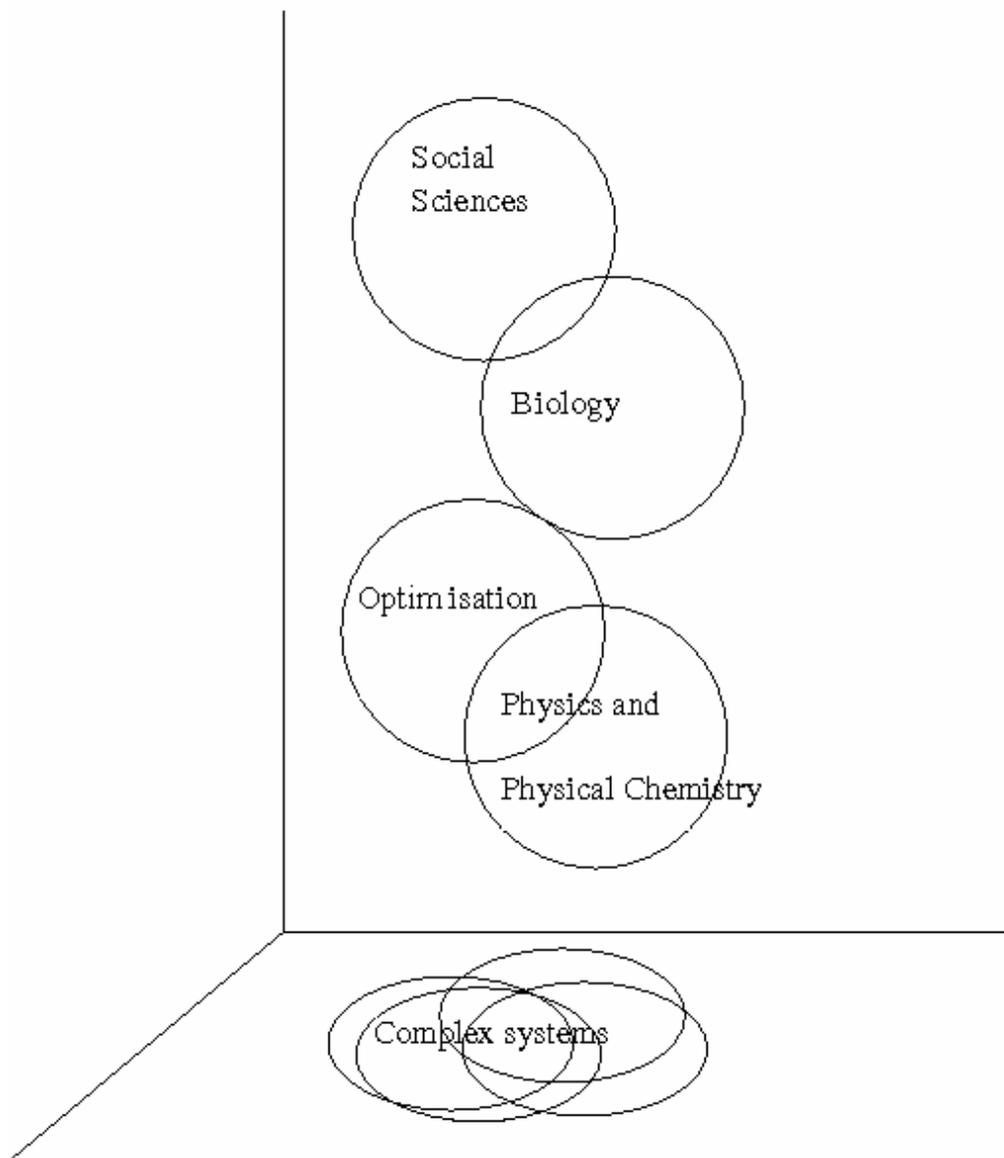


Figure 1: The projection metaphor. Different fields of research, say biology, sociology, physical-chemistry, optimization, share many common traits when checked from a complex system perspective; this is illustrated by the large overlap of the two-dimensional projections on the x,y plane of the four spheres in the 3d space. A projection along another axis, say x, would strongly reduce the overlap.

## **1.2 A historical perspective**

Complex systems perspective and methods are roughly half a century old. The purpose of these reminders is important in the present context: we have now acquired technical tools to deal with real world complex systems. "Complex systems" is not a buzzword, and the interest in complex systems does not boil down to a bandwagon effect. This implies that practitioners in the different fields of application could avoid re-inventing the wheel by either learning the theory, concepts or methods, or collaborating with complex systems specialists.

One could argue that the first computation in the spirit of complex systems approach is Clausius' virial theorem (1857) relating pressure to individual molecules velocity. Of course the names of Gibbs and Boltzmann who later set the basis of statistical mechanics in the 1860's are more familiar. Let us rather start with the first challenges in the applications to biological problems, in the 1940's.

The two seminal papers in complex systems are sixty years old. They address such issues as:

- What are the logical units necessary to build a self reproducing automation? (Von Neumann)
- What can you do with an assembly of formal neurons? (McCulloch and Pitts)

In other words, rather than discussing "wet biology" they approach the issue from an abstract perspective. Both results are expressed in terms of universality, independent of any physical implementation. Assemblies of formal neurons can achieve the computation of any recursive function (i.e. they are equivalent to Universal Turing Machines). Von Neumann proposed a cellular automaton capable of self-reproduction, and of universal computation. Both papers were based on the concept of networks of automata and their dynamical properties (threshold automata for McCulloch and Pitts, Boolean automata for Von Neumann).

The perceptron is a simple architecture and algorithm allowing a machine (a simple threshold automaton) to learn from examples and classify patterns. It is the first example of a device based on complex systems ideas. One of its variants, the adaline, is still in use to automatically trim modems.

Close to the year 1970, three independent contributions stressed the importance of genericity and universality classes. Thom catastrophe theory, and its variant bifurcation theory, is applicable to macroscopic systems, while Wilson and Kauffman ideas are applicable to microscopic systems. The three contributions established the importance of generic properties and classes of universality, a very new concept at that time. Some properties are common to classes of systems independently of the details of the model. Thom and Wilson concepts apply in the vicinity of transitions (singularities for Thom). In a few words, Kauffman model (dynamics of random Boolean nets) suggests that organization phenomena observed in biology (in his case cell differentiation) are common to large majority of random systems built on some simple prescription. In other words, biological organization might not be the result of a strong selection principle, a radical departure from conventional biological wisdom in the 60's.

During the early eighties, physicists started invading biology, cognitive sciences, etc. (Before that time, their efforts mostly concerned the discovery and application of complex systems to phase transitions and to the physics of disordered systems). Hopfield model of associative memories was influential in bringing physicists to cognitive sciences. Kirkpatrick approach to optimization problems through the simulated annealing algorithm inspired from statistical mechanics concerned applied sciences (e.g. chip placement and wiring in computer design). Parisi replica solution to the spin glass problem is an example of the bold simplification of the original problem associated with sophisticated formalism to get formal solutions of very difficult problems. The early eighties are also the time when computers became inexpensive and widely available for simulations. Easier

numerical simulations helped to bridge the gap between observations and experiments on the one hand and simplified theoretical models on the other hand.

The development of cognitive sciences since the mid 80's is probably a general scheme followed by several other disciplines. Two major factors were critical in the shift from psychology to cognitive sciences: a fast development of experimental techniques (intra-cellular recordings, psycho-physics, and later, imagery) and the development of theory (neural nets).

An analogue development, also based on the availability of empirical and experimental data, is the case for the study of financial markets (in the 90's) and of the internet studies (2000's), system biology (biochips in the 2000's), etc.

Applied science domains also flourished since the 80's, implying large communities of scientists: signal processing (artificial vision, speech recognition) and combinatorial optimization.

Beacons in the history of Complex systems

1940's	Mc Cullochs/Pitts Formal neurons Networks eq. to Turing machines	Von Neumann Self reproducing automata	
1950's	Perceptrons (Rosenblatt, SRI)		
1970	Kauffman RBA Generic properties	Thom Catastrophies Structural stability	Wilson RG group Classes of universality
1980	Parisi the replica method	Hopfield Neural nets	Kirkpatrick Simulated annealing

Figure 2: A short historical perspective in complex systems

## 1.3 Concepts and methods

Is there a complexity science? The question is often asked, but the answer depends largely of what is meant by complexity. If we restrict the answer to complex systems, the answer is definitely yes, we have built a theory of complex systems. We will review very briefly in this section a set of concepts and methods which give us a better insight of real complex systems.

### 1.3.1 Concepts

Among the most important concepts are the notions of

- Scaling: Scaling laws can be considered as a first level in modeling; they relate two quantities by rules such as:

$$Q \propto L^\alpha \quad (1)$$

where  $L$  is a parameter (e.g. a length or a number of agents,  $Q$  a dynamic quantity (e.g. a period, some degree of complexity) and  $\alpha$  some real number. The concept is pervasive in all sciences but its importance in complex systems is due to two reasons:

- since understanding complex systems is so difficult, knowing how things depend on each other is already an important result;
  - scaling laws are often generic; genericity is itself an important concept which states that some results are robust and do not depend upon details.
- Universality, genericity. Because the full description of real complex systems is very complicated (in other words of large algorithmic complexity, necessitating a long description), a modeler cannot a priori be assured that the necessary simplification of his model would not change the behaviour predicted by the model. Rather than trying to reproduce all the details of a real system one looks for classes (of universality) of systems which share the same set of properties: the generic properties.
  - Attractors: complex systems evolve in time towards a restricted set of configurations, called attractors of the dynamics. The nature of the attractors (fixed points, limit cycles or chaos), their number, etc. characterise the dynamics. The notion of attractors is the answer to the "Emergence paradox": the system displays some form of organization apparently unpredictable from the rules that specify it.
  - Robustness: the attractors remain qualitatively unchanged over a finite range of parameters, defining a dynamical regime. But sharp transitions in the space of parameters separate dynamical regimes. These properties, dynamical regimes and sharp phase transitions, are the generic properties of the dynamics. Because the conclusions of complex systems studies are about the attractors, they are generic: they are common to large classes of equivalent systems, which may differ in their details.
  - Networks: The concept of an interaction network is central to complex systems. The study of the static structure of the interaction network was recently renewed by the ideas of "small world" (Watts and Strogatz) and of scale free networks (Barabasi and Albert, see further section 4.2). Many empirical studies on real world nets, whether biological (from food webs to gene regulatory networks) and

social (from small communities to WWW) were done in recent years; new characterizations of networks have been proposed and in some cases a bridge was re-established between network sociologists and complex system scientists, e.g. in the search for small motifs in relation with functional properties for instance. Dynamics and functional organization studies are far more difficult to achieve; they also require larger data sets. The predictions of Vespignani et al. on virus infection and immunization strategies in scale-free networks are a good example of the importance of dynamical studies (see further section 3.5).

- Many other general concepts were introduced such as percolation, fractals, self organised criticality, order parameters and functions, etc.

These general concepts guide research on any particular complex system: they are part of a theory of complex systems as the concepts of energy, temperature, entropy, state functions, shape thermodynamics... The analogy was first stated by Stuart Kauffman ("Waiting for Carnot").

### 1.3.2 Methods

In quantum mechanics e.g. computations are based on a series of techniques (e.g. group theory, eigenvalues and eigen functions, perturbation methods). The same is true for complex systems. Let's enumerate some formal techniques:

- Discretization, of time and/or space, e.g. cellular automata.
- Computation of the Z function via the replica ansatz.
- Renormalization group.
- Transfer matrix.
- Random matrices.
- Damage spreading methods.
- Langevin equations.

When formal methods are not applicable, numerical simulations can be used. But complex system methods are not restricted to computer simulations as sometimes stated. The idea is rather to couple formal methods on the simplest models and computer simulations to check the genericity of their conclusions on more elaborate versions.

Computer simulations are often based on methods inspired by the complex system approach to physical and biological phenomena:

- Probabilistic methods such as simulated annealing rather than exhaustive searches in NP complete optimization problems.
- Learning methods such as the perceptron algorithm and its generalizations inspired from neural nets.
- Genetic algorithms and their variants.
- Ants algorithms ...

The complex systems galaxy  
(multi-dimensional aspects)



Perspectives

Descriptive  
Physical, biological, social systems

Normative, design  
Public health, drug design, transportation, governance

Figure 3: Perspectives in complex systems

## **1.4 Caveat: to be transversal or not**

By François Képès

It is a common view among complex systems researchers that their science addresses issues that are fundamental to complex systems in general, starting from important open questions relevant to many domains, and searching for methods to deal with them. In the following, this will be called the transversal approach, as it transversally crosses many disciplines.

The transversal approach has proven its value at the methodological level, and various fields of application have benefited from it. However, its indiscriminate application could potentially lead to failure to recognize the diversity and richness of the applications ('all networks were born equal'), instead of using this richness to improve the transversal approach.

Here we suggest that there are other possible paths to the science of complex systems. In particular, we propose an alternative path that starts from a field of application, and subsequently raises increasingly theoretical and wide-ranging issues. The starting point would be a case study that exemplifies many challenges in complex systems research, for example elemental heterogeneity, interconnected scales in time and space, emergence of higher level behaviour. In a second stage, the analysis of this case study would inspire multidisciplinary research. In a third stage, the challenge of the complex problem offered by this case study and surrounding multidisciplinary approaches, and of large data sets, would attract excellent theoreticians. These theoreticians, in trying to build novel theoretical frameworks and novel concepts from this rich substrate, would uncover specific complex system research tracks, therefore valuably contributing to this science.

## **1.5 Domains of application**

We will develop in the following sections, examples of applications of complex systems methods to several fields of research and development. This set of examples is not meant to be exhaustive: it reflects the availability of experts in these different fields of research, and the timeliness of these topics. The convergence of issues is reflected in the plan of these contributions:

- The different domains have a long history of research previous to the complex system approach; we briefly recall the more standard approaches and their limits.
- "Gaps". Quite often the research communities are partitioned between specialists of the microstructure (or the individual components) and specialists of the collective aspects.
- The success stories of the application of complex systems methods to the particular field of research.
- The future challenges for complex systems methods.

Because complex systems studies are based on the same set of methodologies, the general perspective reflects many commonalities across domains. For instance:

- It is often the case that the success stories relate to theoretical results obtained on non-structured systems, thanks to mean field or related structure methods. While the future challenges concern the application of reverse dynamics to large data sets in biology (e.g. gene regulatory networks), economics (financial markets), etc.

- The importance of networks is pervasive in all domains. One contribution, by Guido Caldarelli (see further section 4.2), summarizes the most recent progress in networks characterization and dynamics.
- In several domains the individual moves are recorded for large ensembles (in the thousands) in order to track the elementary processes responsible for interaction:
  - in ethology of animals groups such as schools of fish, swarms of insects or birds,
  - walkers in crowds,
  - in economics, traders on financial markets,
  - email exchange inside a given community,
  - even in embryology, individual cells of the zebra fish are recorded during ontogenetic development.

These huge recordings have necessitated new progress in tracking algorithms, not to mention the hardware needs.

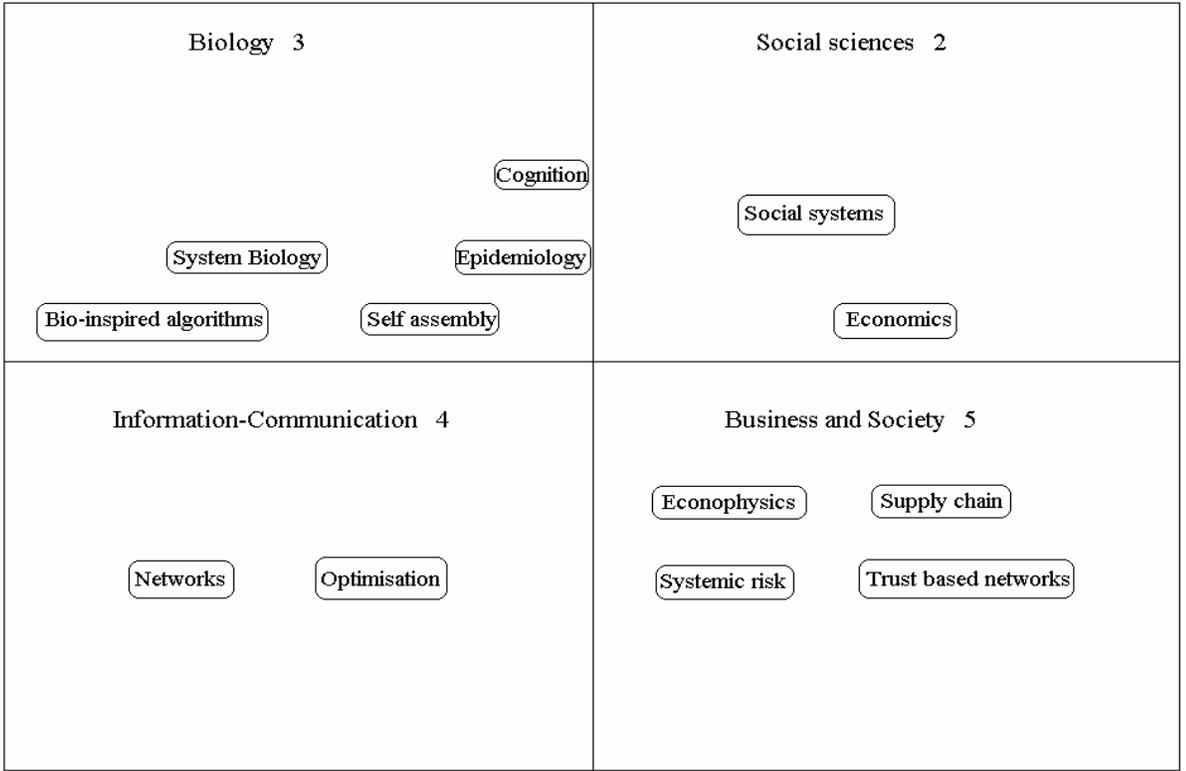


Figure 4: A plan of this brochure

## 2 SOCIAL SCIENCES

### 2.1 Social systems

Social systems are recognised as complex by most modern researchers in the social sciences, but sociology and political sciences are for historical reasons among the less penetrable fields of application for complex system scientists (economics will be later described).

What can a complex system perspective bring to social sciences? Since Max Weber (1864 - 1920), a dominant paradigm in the research program of social sciences has been methodological individualism: how to explain social phenomena from individual rationality. This view is commonly shared in sociology or economics, but its connection to complex system research is accepted, and used, by a minority of social scientists, e.g. Kirman in economics, Axelrod in political sciences (and the BACH group in Ann Harbor, Michigan), Epstein, Axtell and P. Young (the Brookings Institution) in political philosophy and economics. In Europe, Gilbert and Conte e.g. are active in "simulating societies".

The equivalent problem to functional organization in biology is the problem of institutions in social sciences. In a bounded rationality perspective, institutions allow societies to meet the challenges that they face. Social scientists, and not only structuralists, recognize that some social organization allows individuals to act in society. There are many kinds of institutions, from what we obviously recognise as institutions such as schools, hospital, state, law, religions ... to less obvious instances such as cultural traits, routines, etiquette. Even language can be considered as an institution.

Many questions have been asked about institutions but a central issue is the origin of institutions: how do individuals in a society "choose", adopt and maintain institutions? How do institutions evolve? What makes people abide or not by social norms?

The complex system approach as developed by Axelrod, Epstein, Axtell, etc. interprets institutions as the attractors of the dynamics of interacting individuals. Axelrod for instance has launched the research program on the emergence of cooperation in a prisoner dilemma framework. Along this line of research, Epstein and Axtell discussed the emergence of a class system among social agents with a priori neutral labels. Luc Steels demonstrated the emergence of a common vocabulary among a set of communicating robots ("talking heads").

Interpreting institutions as attractors of the social dynamics among agents explain their emergence, their stability and robustness, and the fact that the history of institutions follows punctuated equilibria. If we think of social regimes in societies, one gets an explanation of long stasis of organizations such as tribes, chiefdoms or modern states; transitions among such metastable regimes occur fast and bring very different organizational forms ("revolutions").

Another line of research, also following complex system methodology, is the search for scaling laws in social systems. Quantitative approaches to social systems started with scaling laws (Pareto, Levy, Zipf) reflecting the abundance of structures according to their size. Zipf's law for instance established that the distribution of the size of cities roughly follows an  $1/\text{size}$  law (1920's). The same kind of scaling was observed in the distribution of individual wealth, income, frequency of words in large corpuses, as in natural systems such as earthquakes or climatic events. They imply that there does not exist e.g. a city of "characteristic size" as would imply a normal distribution. The same scale free behaviour is observed in financial time series of returns or in firm size distributions.

Since the pioneering works of Simon and Mandelbrot we have a simple explanation of the origin of these scaling laws: a simple random multiplicative mechanism such as "riches get richer" suffices to yield power law distributions.

A complex system perspective offers many opportunities in the most fundamental aspects of most social sciences. A few examples:

- Language. One is looking for threads to answer questions about the origin and diversity of human language. Not only in terms of vocabulary, but also grammar. Why do we have a limited number of grammatical markers systems among the variety of human languages and why those? The challenges of linguistics and its applications to translation, information retrieving, human/computer communication and communication protocols are of tremendous interest to the European Communities.

- Economic geography. Differences in economic activity, and especially in Europe, are striking; it is a major challenge to European construction (of course the same can be said about cultures). In what respect is economic differentiation due to physical geography or to history? How much differentiation is "natural" or inevitable, because driven by economic growth itself and its aleas (see further section 2.2.2). Understanding cities, growth, shape, interactions, evolution, etc. in connection with their inhabitants' challenges, abilities and individual choices is a typical challenge of economic geography. Many problems call for a complex system approach such as modeling land use, for which cellular automata approaches have been developed.

- Economics (see further section 2.2.2). More generally economics calls for complex systems methods and ideas as proposed by Nobel laureates in economy (K. Arrow) and physics (P.W. Anderson) and D. Pines ("The Economy as an Evolving complex system" 1987-8). With such "founding fathers" and followers this research program soon developed in the US (B. Arthur, SFI) and in Europe (the WEHIA conferences involving e.g. M. Gallegati and A. Kirman). Another factor which has facilitated these developments is the prevalence of mathematical culture among a large fraction of economists. But some tensions and competition with physicists (the econophysicists) and their contribution remain.

- A second area which has been very successful is cognitive science, where complex systems methods helped to establish bridges between the (wet, biological) brain and cognition (see further section 3.3). The fast development of cognitive sciences in Europe since the mid 80's is due to the conjunction of two factors: the use of complex systems methods (especially neural nets) and new recording and imagery techniques (multi-recording, MRI, etc.)

Because of barriers to inter-discipline communication the progress has been much slower in areas such as sociology, political sciences, political philosophy and even management. There exists some interest for complex systems among some scientists in this disciplines, but most often for some "softer" versions.

- In the case of social sciences in a wide sense (including e.g. political philosophy and political science), the chosen methodology is most often numerical simulation with little interest for complex systems concepts. This often translates into bringing all possible knowledge as input to the model, running the simulations (often under multi-agents ideology and platforms), and observing temporal or spatio-temporal patterns. This line of research has been active for more than ten years in Europe ("Simulating societies" with leaders such as Nigel Gilbert, Rosaria Conte, and Andrzej Nowak). Applications to present social challenges such as environment have been a strong incentive for these simulations. They are often developed in institutions closer to applications such as agriculture or halieutics rather than in inner academic circles. By contrast, some physicists (Dietrich Stauffer, Serge Galam, Sorin Solomon, Gérard Weisbuch...) applied complex systems methodology.

- In the case of history, political philosophy and even in management, the softer (rather verbal than modeling) version of complexity is most often used: Edgar Morin in France is an example. These communities often relate to cybernetics.

## Normative approaches and design

Many applications of CSR concern priority areas of European research defined by the Commission such as health, governance, environment, etc. In all these concrete challenges the picture involves on the one hand hard scientific knowledge either in medicine, climate, economy, and on the other hand choices by many inhomogeneous

agents with incomplete information. The agency, EC or national government, has to extract information from a huge set of data, define a policy acceptable for its constituents and implement it. Any help in the different steps of the political action is awfully needed: from data to knowledge, defining a policy taking into account the conflicting requirements of production, environment and social needs, and imagine those measures acceptable by the constituency and helpful in bringing the state of the world chosen by the political level.

All tools and methods of complex systems research are needed to get an integrated assessment of the issues and possibilities. A major challenge for complex system research is to be associated to search for solutions to these societal issues. If we for instance take the case of global warming, the communities of climatologists and economics developed sophisticated models of climate on the one hand and of economics on the other hand. But the integration of these models to achieve some useful assessment has been terribly hard and unsuccessful.

A challenge that is faced both by the scientific community and by funding agencies such as the EC is how to have projects in the priority areas of European research which bring together complex system scientists and specialists of the fields of application, whether agriculture, economics, medicine, etc.

## Design

The scientists' vision of design starts taking into account the fact that designed objects are to be used by humans (of course sellers already understood that, but for them users are only possible customers). The idea of human usage of technical products makes even more sense in our present well connected societies. In the connected society, the success of any communication device largely relies on human factors which might overcome technical strengths or weaknesses. More than ever, innovation means finding new use for sets of technical components that can be either already available or which development can be programmed. Research programs of the IST division are well aware of the importance of these human factors and of the fact that a large part of innovation is driven by communication or based upon the development of ICT. The parallel assessment document for the IST division should be more explicit than ours about challenges and opportunities in IST.

Resource allocation problems are a set of familiar problems in Operational Research (see further section 4.1). But new challenges in our present society such as local decision and the necessity of fast adaptation call for new algorithms. Supply chains methods for instance have to be re-adapted because of the large variability of consumers demand: supplying local dealers with black Ford T in the 20's is a different challenge than supplying the specific model (in terms of colour, motorization and other options) requested by a 21st century customer. Scheduling cannot be completely made in advance and has to be adaptive (see further section 5.3). The "Federal Express" problem is a paradigm of many scheduling problems encountered today, from routing messages along the Internet to handling natural catastrophes: what are the best algorithms to allocate vehicles collecting letters or parcels according to received calls? Simple local optimization algorithms have been invented which parameters are adjusted according to past history of calls. The research community, and especially computer scientists, is more aware of applications in distributed computer science, but many other sectors in business administration call for local and adaptive approaches to resource allocation and scheduling.

In a society where services represent the largest part of the economic activity, a better adaptive allocation is a real challenge which is seldom met (think for instance of the medical services crisis in Europe). One gets the impression that the new developments in the field do not percolate to business through consulting firms or business schools which should be the normal channels (with fortunately some exceptions, see further section 5.6).

## 2.2 Economics

By Mauro Gallegati, Peter Richmond and Massimo Salzano

Everyone would agree that the economy is a complex system. Traditional economics is already a very formalised approach to economy.

Adam Smith, in 1776, proposed that the economy is a complex self-organizing system governed by an 'invisible hand'. This idea of self-regulating order emerging from interactions between elemental components without it "being part of their intentions" became a guiding principle of human behaviour. The approach was transformed in 1870 into a 'theory of General Equilibrium' (GE) by Léon Walras. He proposed a system with a configuration of prices and action plans such that all agents can carry out their chosen plans and markets clear. As this theory was generalized modern, neo-classical, economists seeking to build micro-foundations for macroeconomics soon reverted to the refinement proposed in the 1950s by Arrow and Debreu. They showed that individual agent inter-temporal (on an infinite horizon) optimization also yields a GE, as soon as each representative agent (RA) that makes up this economy is equipped with perfect price foresights for each future state of nature and a complete set of Arrow-securities markets, all open at time zero and closed simultaneously. Whenever these conditions hold true, GE is an allocation that maximizes a properly defined social welfare function or, in other terms, the equilibrium is Pareto-efficient (First Welfare Theorem).

The "gaps": the failure of the micro-foundation program based on representative agents is one. The flaws in solutions to this problem adopted by mainstream macro-economists are pervasive and well known:

- GE is neither unique nor locally stable.
- The GE solution is not computable. Indeed it is not even possible to approximate the system state without going through a full simulation of the actual exchanges occurring in the system. The same problem applies to the class of so-called Computable GE models.
- The GE model is one in which price formation precedes the process of exchange, instead of being the result of it. Real markets work the other way round and operate in real time. Thus the GE model cannot be considered to offer a realistic explanation of economic phenomena.
- It is widely recognized that integrating money into the theory of value represented by the GE model is at best problematic. No individual economic agent can decide to monetize alone; monetary trade should be the outcome of market interactions among agents. By the same token, since credit makes sense only if agents can sign contracts in which one side promises future delivery of goods or services to the other, equilibrium markets for debt are meaningless. Both the information conditions and information processing requirements are not properly defined and bankruptcy, for example, can be safely ignored.
- The only role assigned to time in a GE model is that of dating commodities. Products, technologies and preferences are exogenously given and fixed from the outset. At an empirical level there is an increasing realization that the major economic theories of either Keynes or the monetarist school have not had great success when trying to account for economic behaviour.

The research methodology we endorse in seeking to move forward consists in discarding the Walrasian GE. Instead of trying to deductively prove the existence of an equilibrium price vector  $p^*$ , the complexity approach aims at constructing it by means of rules and algorithms. Clearly, the act of constructing such a coordinated state requires a description of goal-directed economic agents and their interactions.

Agent-based computational economics (ACE), that is, the use of computer simulations to study evolving complex systems composed of many autonomous interacting agents represents an implementation of such a research agenda. With modern computer technology, ACE allows an explicit modeling of identifiable, goal-directed, adapting agents, situated in an explicit space and interacting locally in it. In complex adaptive systems, local interactions between the agents can lead to the spontaneous formation of macroscopic structure not evident by simple consideration of individual behaviours.

Complexity then provides the essential step that takes economics from its position as an axiomatic discipline to being a falsifiable science at the micro, meso and macro levels. It also deals systematically with economic interactions and the aggregation of economic variables.

### **2.2.1 Success stories**

Over 80 years ago in 'Sozial Physik', Lammle showed how social and economic phenomena might be understood by applying simple physical concepts. In the last 20 years the activity of a few has become a global activity with the participation of many groups from across the world. A second motivation for this activity by the physics community has been the availability of an abundance of financial data that now covers activity down to the level of transactions occurring every few seconds. This has allowed empirically inclined physicists with some economists to begin to gain new insights into these markets where trades take place at the level of seconds (Stanley, Farmer). The importance of this work cannot be overstated. If we can really understand what moves financial markets then much financial pain and misery that affects economies and ultimately the lives of citizens everywhere could be reduced.

However not all markets are of this kind. For example, Weisbuch, Kirman and Herreiner (1998) have studied the markets for perishable foods as exemplified by the Marseille fish market. They showed how a model that involved customer loyalty or preference together with a learning element led to an understanding of price development. This model illustrates the emergence of order in the sense of stable trading relationships together with additional insights into the way fluctuations could break down that behaviour. Such models could have application in the wider context of the consumer society and help traders and industrial businesses with purchasing and pricing strategies.

Other economic problems where we are seeing progress are concerned with aspects of industrial organization including distribution and growth rates of firms (e.g. Stanley), income and wealth distributions (e.g. Chatterjee et al. 2005). Ideas first developed to study population dynamics, by Lotka-Volterra (Biham, Malcai, Richmond and Solomon, 2002) now vie with agent models first developed and applied to molecules (Richmond). Such models are challenging the concept of a simple rational agent and introducing heterogeneous agents that act at the micro level and which when aggregated exhibit behaviour that leads to non-Gaussian behaviour with 'fat tails' and volatility clustering. With modern computers it is now possible to simulate increasingly complex models that incorporate the behavioural characteristics of the interacting agents. This offers new opportunities for the physicist, economist and psychologist to cooperate when working on these challenging problems.

Incomes are now recorded with great precision and frequency in countries such as Japan. Unfortunately in many Western countries, data are not always available in a form that helps neither detailed analysis nor model development. This is unfortunate since it is self-evident that if the structure and dynamics of both incomes of individuals and the profitability of businesses can be properly understood, governments everywhere would be in a stronger position to apply fair and effective taxation policies.

Emergence: a key concept inherent to all these problems and one that taxes the theorist is the question of 'emergence'.

Much more elusive is the notion of intermediate levels (as functional mesoscopic entities). Emergent phenomena are composed of persistent patterns. They emerge from the low-level interactions and their emergence is recognized by the fact that they can be operated on by a separate set of rules. This is the sense in which emergent phenomena define "levels". Analogies with physics might be fruitful. Consider, say interacting electrons in the solid state. In some materials the interactions lead to the formation of closely coupled pairs that give rise to superconductivity at the macroscopic level. Superconductivity is thus an emergent state with properties determined by the electron pairs. Emergence may then be associated with persistence of some kind of 'quasi-agent' that is an aggregate of the underlying agents. This concept of functional mesoscopic entities has been proven fruitful on several occasions under different designations such as motifs of well connected subgraphs in social networks or functional motifs in Genetic Regulatory networks.

## Economic policy issues

RA implies the existence of one equilibrium state given the initial conditions: to choose the "best" policy tool for obtaining a desired end would be quite trivial. By contrast, the characteristic of "emergence" peculiar to complex system implies the possibility of reaching one of many equilibria. This begs the question as to whether history and path of the state vector is important.

If economic policy operates on complex environments, ranging from telecommunication networks and financial markets to ecological to geophysical systems, the mainstream tools are, at best, misleading if not inappropriate. Methods developed for linear systems give rise to unintended consequences since implementation of policies can themselves not only change the dynamics associated with heterogeneous agents, but also change the overall landscape within which these agents interact and evolve.

Though the science and technology for the solution of complex adaptive systems have advanced in recent years, their application to economic policy problems seems to have lagged applications to the business and scientific worlds. (One noticeable exception was a simulation of the influence of tic size on the Nasdaq which was not published; the financial sphere is more discreet than the academics ...)

Among suggestions that have been made for controlling complex economic systems:

- It will be necessary to develop a new decision theory based on "robustness" vs. the optimization principle (Lempert, R. J., 2002; Bankes, S. and Lempert, R. J., 1996). J-P Aubin's viability theory (Birkauser Pub., 1991) goes along these lines.
- Ideas of 'control' will have to give way to 'management' of complex economic systems (Rihani, 2004).
- New tools such as those based on 'visual analysis tracing' will be necessary (Shneiderman, 2004) (the approaches of "Exploratory Modelling", Bankes, 1993 and "Adaptive Strategies").

Equally, the strong dependence of complex systems on the initial conditions suggests we shall move away from "high energy control" to "small energy management" of the economy. However, all these ideas and methodologies are still in their infancy and much more work is needed to bring them to maturity.

Specific areas that could be ripe for further analysis and where such new ideas might be further developed at this time include:

- The nature of income distributions and optimum approaches to redistribution within societies.
- Development of tools for identification of the best routes that ensure control of income dynamics during EC expansion and integration of new member states.

- The characterization of financial instability within networks of firms, banks and other organization (see section 5.4).
- Methods for the control and evolution of trade and income distributions across nations.

## 2.2.2 Socio-economic networks

By Gérard Weisbuch

Since socio-economic networks constitute an institutional structure allowing production and trade, their investigation lies at the interface between social sciences and economics.

The concept of networks is pervasive in Complex systems: after all, any interaction structure implies a network. Social networks as a vector for the propagation of information and decision among individuals are an old topic in social sciences since the 40's. It has been active since that time and the Sunbelt Conferences now have participation in the thousands.

The interest in socio-economic networks, where vertices are firms, is more recent and might have arisen from the Asian credit crisis of the late nineties. It contrasts with standard economics which:

- consider firms as independent entities interacting with customers only through the market (General Equilibrium Theory)
- or discuss strategic interactions among a small set of firms (Game Theory).

In both cases, the approach, based on full rationality of economic actors is a search for equilibrium. In real life, firm dynamics are far from equilibrium, and their interaction structure is much more complex than the hypotheses of General Equilibrium or Game theories.

Firms interact via many possible channels, which constitute as many edges of firm networks:

- The most straightforward B2B interaction is through production: the output of a firm is used as an input by other firms.
- Firms also have capital cross-participations or credit relations.
- Firms interact via their personnel: they can share directors on their boards; exchange of professionals is also important in certain industries such as innovation or the media industries.

Industries are shaped by these interactions, especially new industries; understanding the consequences of these interactions is of fundamental importance for producers, investors, banks, national or international agencies.

Many recent studies concerned the static interaction structure describing firm networks. Power laws scaling describing firm size and wealth, as well as their connection structure were empirically observed from public data obtained for instance from stock exchange.

The scale free structure of firms connectivity, -namely the fact that some firms are far more connected than others- whether it concerns trading relationships, partial ownership, sharing directors, etc. already gives a lot of information on strategic interactions and power relations.

As in most network studies, the following issues are addressed in dynamical studies of economic networks:

- How "smooth" is the dynamics? Should one expect equilibrium or some kind of laminar flow of production across the network? Or a richer structure with cycles,

burst of activities, avalanches... Our experience of the real world (business cycles, bursts of volatility on the stock market, bubbles, etc.) evokes unstable dynamics, as opposed to standard views of economics, which discuss any irregularity as driven by external factors (the so-called exogenous shocks).

- How is economic activity and wealth distributed across the net? Are any patterns observed? What is the stability of these patterns?
- Avalanches are among spatio-temporal patterns of interest: they concern avalanches of production events in production networks seen as generalised supply chain, but also propagation of innovations or of bankruptcies.
- "Meta"-dynamics of the network: how is the network structure itself evolving as a function of the business that it supports? What is the role of orders and actual exchanges on the growth and decay of existing links or in the emergence of new links?

A number of these issues were raised in evolutionary economics, in practice mostly concerned with innovation and its interplay with firm economics; or in geographical economics: how to explain the strong localization of economic activity? The localization issue was soon brought to the attention of the observers of the industrial revolution, but the tremendous re-enforcement of localization with the New Industries makes the topics very relevant.

Another domain of economics which should be enlightened by the network approach is the theory of the firm. Although firms are the most important actors of the economical world, we still don't have formal model(s) of the firm. For instance, the mere existence of firms is simply explained in standard economics by transaction costs: a firm with its permanent structure is more efficient than a labour market where entrepreneurs would hire workers on a project basis because of the costs associated with hiring and firing workers. The case of firms is typical of many problems where there exists a deep gap between the approaches used by different scientific communities; in this particular case economics, management science, sociology.

The meta-dynamics of production networks where links are evolving according to business transactions is a rich dynamical path to a theory of the firm. Network vertices can be interpreted as production units; the evolution of some edges towards strong and stable preferential links can be interpreted as merging and acquisitions. Loosening and decreasing relative strength of a link as outsourcing.

All these scientific challenges are fundamental issues faced by modern economies.

## Bottlenecks

The most important present bottleneck is access to individual business transactions. It is connected with the gaps between academics and the private practitioners of firm management, financial officers, consulting firms and even, to a certain extent, business schools.

## 3 BIOLOGY

From the early days of complex systems research, in the 40's and 50's, biological systems were considered as an inspiration for the design of complex artificial systems. But of course, understanding the self-organization properties of biological systems was itself a major challenge.

We will not describe here in detail the bio-inspired applications such as the many applications of neural nets research to signal processing: the reader might check Mark Buchanan's document, or the standard literature on neural nets. We similarly skip DNA computation, immunocomputing, etc. Bio-inspired algorithms will be used in section 3.6.

We will rather concentrate on complex system research motivated by the understanding of biological systems such as cognition, genome expression, the immune system and ecology. This basic research, often referred to as systems biology, poses fundamental scientific questions; furthermore, its application to health, medicine, drug design and environmental issues is of the highest importance. For instance a better understanding of the interactions that control gene expression would considerably facilitate the design of new drugs, both in terms of inventing the drug and synthesizing it, but it would also help to check for possible negative side effects.

The year 2000 has been a turning point in the application of complex system research to biology.

### 3.1 Theoretical biology

By Gérard Weisbuch

Before 2000 the major effort was the understanding of functional properties of biological organs: for instance how can neuron assemblies give rise to cognitive properties in the brain? Hopfield 1982 PNAS paper on associative memories of assemblies of formal neurons is a typical example. Hopfield demonstrated formally that sets of formal neurons educated by a simple delocalised algorithm, Hebb's rule, could later recognize the patterns they had been taught; this recognition does not even request a presentation of the original pattern: even a presentation of a part of the pattern would suffice.

Most of the research of the 40's to year 2000 was along these lines:

- The cellular automata of Von Neumann were proposed as models of self-reproduction.
- S. Kauffman (1969) modeled phenotypic expression based on interactions among gene expression;
- R. Thomas, M. Kaufmann, A. S. Perelson et al. from the 70's modeled the immune response as a result of idiotypic interactions among antibodies and cell receptors.
- A large fraction of the research interpreting the origin of life (Eigen, 1972; P. W. Anderson, 1983; S. Kauffman, 1989) as due to the emergence of a set of autocatalytic polymers belongs to this line of research.
- The gradualism/catastrophism debate. Punctuated equilibria (the genotype/phenotype/population dynamics).
- Population ecology (Red Queen paradox, co-evolution, game theory and replicator dynamics, massive extinctions seen from the Self-organised Criticality perspective).

At that time, the complex systems approach was an alternative to the reductionist approach which considered biological functions as the result of a finely tuned selection and pruned a major effort at specifying the details of all involved components and of their interactions. The complex system scientists established that functional properties could be the result of interactions among rather simple entities. Functional organization was shown to be a generic property of the attractors of the dynamics of the interacting system rather than the result of highly tuned natural selection. These earlier efforts greatly improved our insight in biological organization.

### **3.2 Systems Biology**

By François Képès

Standard approaches and their limits

Molecular biology, a field initiated and developed by the interactions between biologists, biochemists, mathematicians and physicists, has provided a wealth of detailed knowledge about molecular mechanisms at work in organisms. Most recently, the contributions of computer scientists have enabled breakthroughs in the acquisition and interpretation of genomic data. As yet, however, none of these critical achievements has allowed us to obtain an integrated understanding of the functional modules and regulatory networks involved in cell and organismal physiology.

The promises raised by the identification of genes involved in multifactorial diseases have not turned into efficient therapies because most molecular biologists have focused on individual genes and proteins rather than on systems, and have not addressed questions such as:

- What is the functional architecture of these interaction networks and their modules, what are their dynamic properties? How do different levels of regulation intermingle? What are the organizing principles at play?
- How do robust behaviours emerge amidst stochastic molecular events?
- How is the expression coordinated of genes involved in the same physiological process?
- How do cells tolerate, control or use noise in regulatory networks?
- How has evolution shaped these networks?
- How can results obtained in model systems be used to improve human therapy?
- How can regulatory networks be deciphered in a way that would allow the diagnosis and prognosis of multifactorial diseases and the design of new therapeutic strategies?

In order to tackle these questions, biologists, physicists, chemists, computer scientists and mathematicians are needed. Together, they pave the way to a new approach in life sciences dubbed "systems biology". This renewal of integrative approaches in biology takes its roots in the legacy of quantitative and theoretical biology, and in the conceptual developments on self-organizing systems in the 1980's. In the past 10 years, it has been fueled by the availability of huge datasets produced by the "-omics" methodologies. As these methodologies are the daughters of biochemistry and molecular biology, the datasets have a marked molecular grounding, hence the molecular slant of systems biology in comparison to its ancestors.

As an emerging discipline, systems biology cannot and should not be defined in a strict way. Rather, it should be defined in an epistemic way, as a set of successful approaches that, together, constitute the first landmarks on a virgin territory.

## Gaps

Several types of gaps must be considered in the case of systems biology.

The first one is cultural. Several scientific communities must closely interact for success, from bench-work to theoretical biology, the latter often being held in suspicion by bench biologists. For most molecular biologists, modern biology roadblocks are on the experimental side, while the vision from Systems Biology is how to build biological insight and transferable knowledge from a huge amount of experimental data. Still, to cut down on costly bench-work, it would probably be a good idea to organize and improve the synergy between conventional and computational experimentations.

The second gap is ontogenic. One of the major challenges ahead of us will be to make the best use of the massive amount of molecular data generated by the tools of post-genomics. It is clear that the abundance of such data has increased tremendously in the recent past. Yet a closer look reveals that, with the exception of genome sequencing in most cases, such data are not truly exhaustive, and their quality is generally poor, although slow improvements can be foreseen. Thus, for a long time to come, the lack of exhaustivity and the poor quality of the data will be a serious ontogenic obstacle to quantitative predictions. Other approaches may sometimes permit one to make useful predictions from qualitative or semi-quantitative results. Importantly, it often suffices to be able to give the evolutive trend of the final parameter to determine the outcome. For example, if spontaneous cell death outweighs division in the tumor cell, cancer will regress, which is the single most important fact. Besides, it would be wasteful to convert the few available quantitative data into qualitative results for the sake of format homogeneity. It will therefore be crucial to succeed in combining, in the same simulation, the use of quantitative and qualitative results.

The third gap is epistemologic. The temptation to build a cell and an organism from their genomes and related molecular data implicitly relies on the conception that all the cellular information lies in the genome. This viewpoint is not warranted by available facts, yet it is widespread, thus creating an epistemologic obstacle. An obvious counterexample is that two human cells endowed with an identical genome may exhibit extremely different phenotypes (compare, for instance, a stomach cell and a neuron). It is thus clear that part of the cellular information is held in its genetic material, while another part is distributed elsewhere in the cell. The genetic information is easier to identify, as it is contained mostly in one DNA molecule and is relatively accessible to us in the form of the genome sequence. This may explain why the genetic part is so strongly emphasized.

## Success stories

Expectedly, there are few success stories in such a recent field of investigation. Yet, three examples will illustrate a variety of potential approaches. However, let us first sketch some landmark developments in this field.

The first surprise came when it was demonstrated that biological systems ranging from food webs in ecology to biochemical interactions in molecular biology could benefit greatly from being analyzed as networks. In particular, within the cell, the variety of interactions between genes, proteins and metabolites are well captured by network representations and associated measures including degree distribution, node clustering, hierarchy and assortativity (Barabási and Albert, 1999; Ravasz et al., 2002; Watts and Strogatz, 1998). The global topology of these networks showed similarities among themselves as well as with respect to sociological and technological networks (Jeong et al., 2000; Guelzim et al., 2002; Shen-Orr et al., 2002).

In a second step, the issue of local topology, subgraphs and motifs was addressed. A number of biological networks were found to contain network motifs, representing elementary interaction patterns between small groups of nodes (subgraphs) that occur

substantially more often than would be expected in a random network of similar size and connectivity. Theoretical and experimental evidence indicates that at least some of these recurring elementary interaction patterns carry significant information about the given network's function and overall organization (Guelzim et al., 2002; Shen-Orr et al., 2002; Milo et al., 2002; 2004). Feed-back loops, feed-forward loops and other motifs were thus uncovered in real-world networks, and were attributed a qualitative dynamics.

In a third step, such dynamics were shown to be effective by monitoring them in a synthetic network with the same topology that had been implemented in live cells (early attempts: e.g. Becksei and Serrano, 2000; Elowitz and Leibler, 2000). In reverse, network design could be automated by evolution in the computer towards a fixed goal such as behaving like a toggle switch (François and Hakim, 2004).

The following two examples illustrate successes using the discrete and differential approaches, respectively.

The first example testifies to the usefulness of a discrete logical approach relying on few available data and drawing from the corpus of formal methods from computer science. The bacterial population that opportunistically invades the lungs of patients afflicted with cystic fibrosis often switches several years later to producing mucus, thereby becoming more resistant to antibiotics and making breathing more difficult for the patient. Two hypotheses with different therapeutical prospects, genetic and epigenetic, have been proposed to explain this mucoidal switch. The generalized logical method proposed by René Thomas, coupled to temporal validation (Bernot et al., 2004), allowed to validate plausible models and to formulate the most discriminatory experimental plan for choosing among the genetic and epigenetic hypotheses to explain the mucoidal switch (Guespin-Michel et al., 2004). The experimental plan has been carried out successfully, with useful feed-back for the model.

Modeling of chemotaxis in bacteria exemplifies differential or stochastic approaches applied to understanding a phenomenon that exceeds human intuition. Chemotaxis refers to the cell ability to swim or move towards a chemical attractant or away from a repellent. The mechanisms of chemo-taxis in eubacteria (Shimizu et al., 2003) and archaeobacteria (Nutsch et al., 2005) turned out to be principally different, although they are both based on a random walk that is biased by comparing the actual chemical concentration to that memorized at a previous time. In eubacteria for instance, the model not only matches experimental observations, but shows an unexpected emergence of spatial patterns of methylation, the chemical modification involved in the memory effect (Shimizu et al., 2003).

A last example shows how the coupling of bench and computer experimentation may provide answers to fundamental questions. Here, the issue is evolutionary optimization of fitness to environment by adjusting a certain protein level. Bacteria were challenged during several generations with various external concentrations of a sugar, and the cellular production of the sugar-metabolizing protein was correspondingly monitored. A predictive cost-benefit model was considered, in which the growth burden of producing the specific protein was balanced by the growth advantage of utilizing the sugar when and as available. In a few hundred generations, cells evolved to reach the predicted optimal protein production level. Thus, protein production appears to be a solution to a cost-benefit optimization problem, and to be rapidly tuned by evolution to function optimally in new environments (Dekel and Alon, 2005).

## Future challenges

Globally, one of the major challenges associated with systems biology is to try and understand the behaviours of biological networks of interactions, in particular their dynamic aspects and spatial developments, often with a goal to later control or even design them. More immediate objectives would include for instance dealing with their natural heterogeneity and size, including spatial aspects, usefully re-composing the subnetwork motifs into a grand network. These challenges typically require cross-disciplinary import of concepts, and crosstalk between experimentations through bench-work and through modeling and simulation.

The success of this emerging discipline will rely upon new techniques and concepts. From the biological perspective, these techniques and concepts will come from areas including the following: - multidimensional and quantitative imaging of molecular events; - modeling, simulating and mimicking signal transduction pathways and regulatory networks both for the conception of experiments and the interpretation of data derived from these dynamic images and from high-throughput techniques; - bio-inspiring evolutionary algorithms, which reflect back into improved biological models (see also section 3.4); - using micro- and nano-technologies to explore, manipulate and mimic the cellular nanoenvironment and to build new bio-sensors.

Big pharmaceutical companies in Northern America, unlike those in Europe, are embarking on systems biology, with various goals that generally include several of the following:

- Personalized healthcare
- Cost-effective treatment (economic benefit)
- Personalized intervention with a model of the patient (individual benefit).
- Model-based intervention strategies
- Combined drug targets (addressing cases where more than one target should be hit at once to reverse the pathology)
- Drug-drug interaction (assessing the combined effects of multiple drug therapies)
- Chronotherapy (process-based time-dependent drug administration)
- Disease reclassification (based on molecular evidences).
- Streamlining therapeutic approval
- Shortening clinical trials
- Reducing animal testing

From a more mathematical point of view, several new techniques and concepts are likely to stem from the so-called "inverse" problem. The availability of huge datasets since the 1990's such as transcriptomes obtained from biochips, multi-neuron recording, and new imaging techniques for instance, opens a new era in complex systems methods. Can we meet the challenge of this data driven biology and extract sensible information from these very large data sets? To be more specific, can we for instance extract the specific sets of interactions among genes which control gene expression in the cell? In mathematics, such a problem is called an inverse problem: rather than finding a trajectory knowing the dynamics governing the system, we here have to solve the inverse problem, getting the dynamics from the observation of successive configurations of expressed genes.

Inverse problems are known to be much harder to solve than direct problems. Moreover, in systems biology one has to solve a problem with a very large number of unknown parameters. Even when supposing that the set of interactions among an ensemble of  $N$  elements is sparse rather than complete, we obtain a number of parameters to be determined that scales as  $N$ . Furthermore, in general, the structure of the network is a priori unknown, and so is the nature of the interaction function.

Fortunately, inverse problems relate to a number of problems already treated in complex systems research. Learning by formal neuron networks is an inverse problem: it simply means finding the set of interactions which associates output patterns to input patterns. Variants include pattern sequence generators. An exciting prospect is to use

and generalise learning techniques to e.g. decode gene regulatory networks using transcriptomic data that provide time series of gene expression levels. Among the methods inspired from complex systems research that can be used to solve this problem, one of the most successful ones in the past years relies on the Bayesian framework (e.g. Friedman et al., 2000). Alternative methods are likely to be evaluated in the coming years, such as genetic algorithms or the survey propagation algorithm developed for constraint satisfaction problems.

Finally, it should be stressed that the development of systems biology will be guided by historical and epistemological analyses of the interactions between biology and other disciplines. It will also be important to recognize the ethical questions raised by the development of systems biology, and to answer these questions by challenging human creativity rather than by dictating laws.

### **3.3 Cognitive Science**

By Jean-Pierre Nadal

Cognitive science is about understanding both natural and artificial intelligence, and requires interdisciplinary approaches. At the intersection of biology and human sciences, it borrows techniques and concepts from many scientific domains - psychology, neuroscience, linguistics, philosophy, anthropology, ethology, social science, computer science, mathematics and theoretical physics. The RIKEN Brain Science Institute (<http://www.brain.riken.go.jp/>) in Japan is one of the best examples of interdisciplinary institutes which have been created in recent years all over the world, with departments on several aspects of cognitive science: Understanding the Brain, Protecting the Brain, Creating the Brain (artificial intelligence, robotics), and Nurturing the Brain (brain and cognitive development). Interdisciplinary laboratories and institutes can also be found in Europe: one may mention the Cognitive Neuroscience Sector at SISSA, Trieste; the GATSBY Computational Neuroscience Unit at UCL, London; the EPFL's Brain and Mind Institute in Lausanne; The Cognitive Science Institute (ISC) in Lyon and the Department of Cognitive Studies at École Normale Supérieure in Paris.

Several important topics in cognitive science are concerned by the field of complex systems. Here are a few examples.

- Modeling and simulating brain functions requires the mathematical analysis of large interconnected neural networks.
- The study of collective behaviour, in social animals and in human societies requires similar tools.
- The analysis of data from brain imaging leads to difficult problems in artificial vision, data analysis, and modeling.

An important complex systems topic concerning cognitive science and many other fields is the one of learning. This name evokes different but related aspects.

- On one side, the theoretical and experimental study of learning and adaptation, at all possible scales: at the cellular level, the network level, the agent level (analysis of human behaviour), at the collective level.
- On the other side, solving inverse problems requires the development of algorithms which can be understood as having a system learning a rule (a function, a task) from examples.

Learning theory, statistical (Bayesian) inference, optimal control, learning in formal and natural neural networks, supervised or unsupervised learning, reinforcement learning, are all different aspects of this same general topic. On the computer science side, the

name Machine Learning denotes this general approach of learning a task from examples making use of any relevant algorithm. Machine Learning is proving an increasingly important tool in many fields, such as Machine Vision, Speech, Haptics, Brain Computer Interfaces, Bioinformatics, and Natural Language Processing. The EU has supported specific actions related to Machine Learning. For instance, the PASCAL network of excellence of the FP6 program (see <http://www.pascal-network.org>) was created in order to build a Europe-wide distributed institute, which goal is to pioneer principled methods of pattern analysis, statistical modeling and computational learning. Combinations of concepts and tools taken from learning theory and statistical physics have allowed to address the modeling of dynamical networks, such as neural networks, genetic networks, metabolic networks, social networks, communication networks... In such domain, one has to both, solve inverse problems (finding the network parameters from the empirical observation of the network activity), analyse and/or simulate the network dynamics, in particular when the network components (cells, proteins, human agents.) are allowed to adapt to the environment and to the behaviour of the other components.

### ***3.4 Engineering emergence in self-assembling systems***

By Norman Packard

Self assembly is the spontaneous organization of components into larger-scale structures. At the molecular level, this process is "automatic", in the sense that the components are driven by the laws of thermodynamics to organize themselves into a minimum free-energy state, which happens to be a complex structure. The molecular domain is particularly powerful and interesting for exploring self-assembly because forces between charged molecules and surrounding substances (e.g. water or other solvents) create the appropriate thermodynamic conditions for complex self-assembly.

Self-assembly is a bottom-up process, defined by local properties of the self-assembling components interacting with each other and their environment. These local properties in turn determine the form of the self-assembled structures, but the self-assembly process may be complex, in the sense that the detailed form of the self-assembled objects is not predictable or derivable from knowledge of the component properties. This bottom-up process is to be contrasted with top-down design processes that specify a target form in detail, and then use a highly controllable process (such as photo-lithography) to create it.

Self-assembly is now recognized as the primary path for the construction of nanodevices. Other approaches based on transporting traditional top-down engineering to the nano-scale, such as a programmable universal constructor envisioned by Drexler, appear difficult for various reasons, including the effects of thermal noise at the nano-scale.

#### **3.4.1 Control and programming of self-assembly**

Given the bottom-up nature of self-assembly, the final product may be difficult, if not impossible, to control if the dynamics of self-assembly process are complex. This is typically the case in self-assembly of amphiphilic structures such as micelles or vesicles, and any time the self-assembly process includes nontrivial chemical reactions.

There are, however, some self-assembly processes that are not complex, and that are in fact controllable to the point that they are explicitly programmable, either by synthesizing polymers (e.g. DNA, cf. Rothmans (2006), *Nature* 440, p. 297) so that they will fold automatically into particular structures, or else by imposing strong boundary conditions on the self-assembly process that determine the final form (cf. D. Dendukuri, D.C. Pregibon, J. Collins, T.A. Aatton, P.S. Doyle (2006) "Continuous-flow lithography for high-throughput microparticle synthesis", *Nature Materials*, April). These processes have

been very successful in producing nano-scale modules, but have yet to become integrated into systems with full target functionality.

The problem of programming self-assembly becomes a true complex systems problem when the components are not strongly controllable, because the self-assembly process has multiple dynamic pathways with strong nonlinear interactions between components. In such cases, the final form of the self-assembled objects is not knowable. Thus, traditional approaches of programming by planning placement of modules explicitly cannot work. Instead, the space of self-assembled objects must be explored by sophisticated search and optimization algorithms to achieve a programming goal.

Examples of complex self-assembly processes include:

- Amphiphilic self-assembly of fatty acids and other lipids into micelles, vesicles, tubes, perforated sheets, etc. depending on constituent amphiphiles and their thermodynamic phase (e.g. work of Luisi, Walde, Sczostak, and Hanczyc).
- Vesicle formation from novel inorganic substances (e.g. Tianbo Liu, Ekkehard Diemann, Huilin Li, Andreas W. M. Dress and Achim Mueller (2003) "Self-assembly in aqueous solution of wheel-shaped Mo<sub>154</sub> oxide clusters into vesicles", Nature 426, pp. 59-62).
- Nanostructures from organic synthesis (e.g. work of G. von Kiedrowski, L. Cronin).
- Surface functionality, either surface energetic or surface patterning, in the context of nano-electronics (inorganic) and functionalized organic molecular layers.
- DNA scaffolding: extensive library of structures formed by DNA, including barcodes, wires, complex matrices for attachment of reactants.
- Nano-gold attached to various structures (e.g. DNA, Rubidium), usable for electronic functionality or local heating of a nano-structure.
- Molecular motors and muscles: components for moving molecules as well as aggregates have been developed at the component level.
- Fused-polymer shapes.

Communities spanned: synthetic chemistry, MEMS (micro electromechanical systems), molecular computing, physics, numerical computation (molecular dynamics, dissipative particle dynamics).

Potential research and application areas: molecular circuitry, computation, molecular robotics, biosensors, energy, artificial living cells.

Future challenges: specific research area targets. These target areas could span research and application areas listed above.

- Extracting electrical energy from nano-objects.
- Extracting mechanical energy from nano-objects (muscles and motors).
- Functionalizing nano-objects by coupling to chemical reactions.
- Achieving multiple functionality with multiple co-existing assembly processes and chemical reactions.
- Programmed interactions with living organisms.

### ***3.5 Epidemic modeling and complex realities***

By Alessandro Vespignani

A wide range of modeling approaches are crucially depending upon the accurate and realistic description of social/infrastructural and behavioural data in spatially extended systems. This includes the movement of individuals at various different levels, from the global scale of transportation flows to the local scale of the activities and contacts of individuals, interrelations among infrastructure networks (cyber/physical levels) and the complex feedback mechanisms regulating traffic and behaviour. These factors are determinant in a wide range of problems related to understanding and forecasting the system behaviour in epidemiology, population biology, transportation and traffic analysis, infrastructure planning and social behaviour.

In this context, mathematical epidemiology approaches has evolved from simple compartmental models into structured models in which the heterogeneities and details of the population and system under study are becoming increasingly important features. In the case of spatially extended systems, modeling approaches have evolved into schemes which explicitly include spatial structures and consist of multiple sub-populations coupled by movement among them. This patch or meta-population modeling framework has then evolved into a multi-scale framework in which different granularities of the system (country, inter-city, intra-city) are considered through different approximations and coupled through interaction networks describing the flows of agents (people, animals, merchandise, parcels of information, technology). In addition, the introduction of agent based models (ABM) has enabled to stretch even more the usual modeling perspective, by simulating these systems at the level of the single individual.

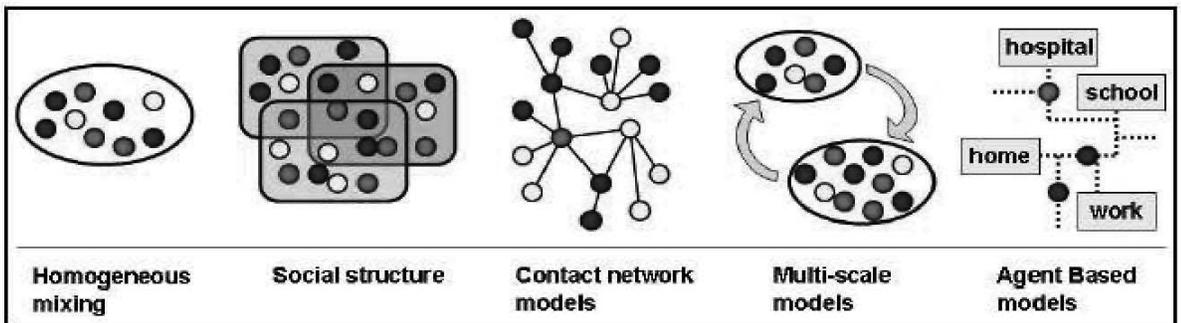


Figure 5: Different scales structure used in epidemic modelling. Circled symbols represent individuals and the different shades of gray correspond to a specific stage of the disease. From left to right: homogeneous mixing, in which individuals are divided into compartments and assumed to homogeneously interact with each other at random; social structure, where people are classified according to demographic information (age, gender, etc.); contact network models, in which the detailed social interactions between individuals provide the possible virus propagation paths; multi-scale models which consider sub-population coupled by movements of individuals, while homogeneous mixing is assumed on the lower scale; agent based models which recreate the movements and interactions of any single individual on a very detailed scale (a schematic representation of a city is shown).

The above modeling approaches are based on actual and detailed data on the activity of individuals, their interactions and movement, as well as the spatial structure of the environment, transportation infrastructures, traffic networks, etc. While for a long time this kind of data was limited and scant, recent years have witnessed a tremendous progress in data gathering thanks to the development of new informatics tools and the increase in computational power. A huge amount of data, collected and meticulously catalogued, has finally become available for scientific analysis and study.

Networks which trace the activities and interactions of individuals, social patterns, transportation fluxes and population movements on a local and global scale have been analyzed and found to exhibit complex features encoded in large scale heterogeneity, self-organization and other properties typical of complex systems. Along with the advances in our understanding and characterization of systems complexities, the increased CPU power has led to the possibility of modeling multi-scale dynamical models by using thousands of coupled stochastic equations and allows agent based approaches which include millions of individuals. This prompts to the definition of a modern computational epidemiology area that integrates mathematical and computational sciences and informatics tools and aims at providing a new approach to the forecast and risk assessment for emerging disease.

Key elements in the development of such an approach are the integration of information technology tools and techniques with the perspective coming from complex systems analysis. By one side this computational approach needs to integrate GIS techniques, on-line data analysis, petabyte data handling and simulations, with the creation of the necessary infrastructures. On the other hand such an approach has to deal with all the complexity features emerging in the analysis of large scale systems made by a massive amount of elements/individuals. Non-linear behaviour, cooperative and emergent phenomena, complex networks, etc. cannot be neglected and will be at the basis of the interpretation and understanding of results as well as in the formulation of the opportune computational techniques.

Meeting this challenge however requires to adapt and complement the basic approaches developed in mathematical and statistical epidemiology to large scale systems ( $10^4$  to  $10^6$  degrees of freedom) and to investigate in a systematic fashion the impact of the various complexity features of real systems on the basic properties of epidemic spreading. In particular this implies filling some major theoretical and methodological gaps. The first one concerns basic theoretical foundations and analytical understanding of multi-scale epidemic models with many degrees of freedom and their interplay with the complex societal networks. What are the basic principles and theory that govern epidemic behaviour in large scale complex multi-scale network and Agent Based epidemic models? How do the large scale complex features (scale invariance, extreme heterogeneity, and unbounded fluctuations) of interaction and communication networks affect the behaviour of spatially extended epidemic models? A further challenge is that even in the assumption that the models used provide an exact description of reality and captures all the features of the system, it is clear that our predictive power will be limited by the impossibility of an exact knowledge of the precise state of the system. In addition, quantitative data on the social response to emergency and crisis are needed in order to have correct epidemic forecast, risk assessment, scenario evaluation. New experiments should therefore be devised in order to provide the correct data driven inputs necessary in large scale simulations.

Despite such an integrated computational approach is still in its infancy, the level of realism and detail achievable today allows us for the first time to ambitiously imagine the creation of computational infrastructures able to provide reliable, detailed and quantitatively accurate predictions for disease spreading. These will be based on real time data collection and large computational models as it is now done in the case of weather forecast. In other words computational approaches are now ready to interface with the complex features of infrastructures and social dynamics, entering the era in which it may become a major predictive tool.

## Grand challenge

Large computational/modeling infrastructure (petabyte-computation, billions individual agents) Modern Computational approaches and infrastructures as sophisticated and effective as the weather forecast approach in modern meteorology. Meeting these challenges requires to adapt and complement the basic approaches developed in mathematical and computational methods, as well as the data gathering infrastructures, to the detailed description of large scale systems ( $10^4$  to  $10^8$  degrees of freedom) and to investigate in a systematic fashion the impact of the various complexity features of real systems on the basic properties of epidemic spreading.

### Intermediate challenges:

- Data collection/integration infrastructures and projects. Quantitative level. Establishment of monitoring infrastructures able to provide a constant output of longitudinal data.
- Next frontier of network science. Theoretical foundations of network interfacing; multi-scale, multi-layer networks understanding; mutual feedback representation. Theoretical and data gathering effort.
- Conceptual (intermediate theoretical understanding). While extremely powerful, however, these numerical tools are often not transparent, being extremely difficult, if possible at all, to discriminate the impact of any given modeling assumption or ingredient. In addition, complexity is not the same as the merely complicated elements accounted for in sophisticated computational approaches. There is a need to investigate in a systematic way the impact of the various complex features of real systems on the basic features of the phenomenon/process at hand.

### Important key factors for success:

- Global effort (multi-country, data sharing)
- Inter-disciplinary effort

## ***3.6 Bio-inspired strategies for new computing architectures and algorithms paradigms***

By François Képès

### Rationale

In contrast to purely technological systems, life forms show a high capacity to self-organize, replicate, grow, heal, adapt and evolve. This is why biology was and remains a major source of inspiration for the design of new hardware, computing architectures, algorithms and software programming paradigms. Such inspiration mostly comes from the following biological processes: evolution, development, and growth. These processes share highly refined regulations but strongly differ in their mechanisms and in their time scales.

Evolution has inspired algorithms that efficiently solve difficult optimization problems. In the past two decades, such algorithms have successfully found applications in science, engineering and humanities. In the field of genetic and evolutionary computation (GEC), as in biological evolution, variation, selection and amplification steps are sequentially repeated to trace a path towards an improved solution to the problem at hand.

Development is not directly encoded by the genotype. Rather, development unfolds in time and space a network of interactions which in turn is orchestrated by genotypic information. Interestingly, this genotypic information is interpreted in ways that vary as the developmental process unfolds and modifies its own environment. Among other things, development is therefore a good inspiration for designing systems with an enriched genotype-to-phenotype mapping.

Growth and cell division constitute a prime example of how a distributed system may operate, bounded only by finite resources. Even in modern cells, division is a process of fracture and stochastic distribution of constituents among the daughter cells. Even large unique bodies in a cell such as the animal Golgi apparatus are broken into numerous pieces before division occurs. The only exception to this rule is the genetic material which is quantitatively duplicated and faithfully segregated. Both this exception and the general process of fracture and growth could be harnessed in environment-sensitive systems such as growing and dividing hardware.

### Present bottlenecks

Examples of bio-inspired computational approaches now span a whole range from behavioural approaches like ant algorithms to molecular approaches like genetic algorithms, genetic programming or artificial chemistries. However, most GEC techniques were designed on the basis of biological knowledge of the '80s and earlier times. In the meantime, biology has brought a wealth of new knowledge that could fuel advances in GEC. Another current shortcoming originates from the fact that genotype-phenotype mapping is still rudimentary in most applications.

### Impact

Past experience with bio-inspiration indicates that this interdisciplinary exploration of self-organization, adaptation, evolution and other emergent functionalities of living systems will further improve our ability to design new computing models, algorithms and software programming paradigms. These improvements will indeed be of a quantitative nature, but a qualitative jump is also to be expected, as the problems addressed by information technology are insidiously bounded by common knowledge of what can currently be tackled. Moreover, there is enormous potential for applying the outcome of this exploration at the physical level, in particular at the nano- and micro-scale, to develop new types of growing and evolving hardware and intelligent materials that could be applied in a variety of ambient interfaces.

### Main research objectives

To tackle problems that were intractable thus far, that are multi-objective, or that cannot even be anticipated, it may be foreseen that algorithms must be complexified. Such future problems share a few features, including the following: they cannot be fully specified beforehand; they vary with time; the relevant data are available but are not sorted from irrelevant ones; the solving process must harness emergence to overcome the "complexity" ceiling; it must not presume human intervention.

Complexification of the algorithms would often involve allowing new degrees of freedom. Merely adding degrees of freedom does not constitute a solution however, as the searching process loses efficiency. Therefore, it is clear that allowing new degrees of freedom should be accompanied by restrictions either in the authorized processes or in the parameter ranges. In this delicate balance between restriction and freedom, bio-inspiration has proven a fruitful guide, and the objective here is to resort again to bio-inspiration to reach the above main objectives.

## Specific objectives

Achieving useful complexification will require research in several directions, including:

- Enriching the genotype-phenotype mapping (e.g. making it emergent) with concepts such as distributed causality or feedback control, inspired e.g. by the sophisticated behaviour afforded by development or individual variability.
- Implementing open-endedness, e.g. where evolution moves its own target, or fitness function evolves.
- Moving from single-objective to multi-objective optimization goals.
- Maintaining a vast repertoire of potential algorithms or solutions and means to mobilize it.
- Implementing a simplified physical model in appropriate cases, e.g. where a micro-dynamics and a macrostructure influence each other.
- Evolving large complex systems from a lineage of less complex systems.
- Continuous data mining from ever growing databases.
- Innovative design involving the creation or deletion of variables.
- Generation of "surprising" hypotheses, bridging the gap with Artificial Intelligence.
- Feature selection in data-rich environments that vary as a result of internal dynamics.

## Timeliness

While an increasing number of bio-inspired optimization methods are now claiming human-superior quality of solutions, while the fields of bio-inspired applications are numerous in science, engineering and humanities, we are still far from tackling real-life complex systems. This research and development will contribute to the design of algorithms and methods that incorporate strategies from the living matter and that can tackle problems that were intractable so far.

## Relevant fields

ICT (optimization algorithms, artificial evolution, artificial intelligence, artificial chemistry), life sciences (molecular biology, cell biology, physiology, systems biology), engineering (optimization).

## 4 INFORMATION AND COMMUNICATION TECHNOLOGIES

### 4.1 Optimization and Complexity

By Rémi Monasson

Optimization is a task of crucial importance in industrial and social processes. Basically the problem is to find the minimum (or the maximum) of a function called cost over a large number of variables. Perhaps the most famous example of optimization problem is the so-called travelling salesman problem (tsp), where a person has to visit a set of towns and come back to its starting point. The cost function is the total length of the tour, the variables are the order (permutation) of the towns to be visited. Another celebrated problem is the constraint satisfaction problem (csp): given a set of logical constraints over, say, Boolean variables, what is the largest number of constraints that can be satisfied altogether?

Tsp, csp, and hundreds of other problems have been studied for decades in computer science. A major result, which emerged in the seventies, is the concept of computational complexity. Problems were classified in terms of the growth of the running time of resolution algorithms. Briefly speaking easy problems are the ones for which there exist algorithms finding the optimum in a time growing only polynomially with the number of data (e.g. the number of towns in tsp, of constraints in csp). The other problems, for which no such polynomial algorithms are known and all known algorithms can take exponentially growing times, are called hard.

This classification has played and is still playing an enormous role in computer science but suffers from some weaknesses. The most important one is that it is a mathematical concept based on the idea of worst case. To be more precise consider again the tsp problem. Tsp is considered to be hard since there is no algorithm (so far) guaranteed to find the shortest tour over ANY set of N towns in a time polynomial in N. But finding the shortest tour can be easy for some, not to say, most sets of towns! In other words the worst case classification can be too pessimistic. Another criticism is that, while finding the true optimum can be hard, it can be much easier to find very good approximations of this optimum, of sufficient quality in practical applications.

Based on these considerations people in artificial intelligence and practitioners as well as theoreticians in computer science have started to study the hardness of optimization problems when the input data are randomly chosen from distributions mimicking as close as possible realistic data or more academic distributions easy to generate (but not solve!) on computers. An important heuristic finding was done at the beginning of the 90's when people discovered the existence of phase transitions, very similar to the ones encountered in the physics of condensed matter, in the problem of Random Satisfiability (sat), a particular case of csp.

Briefly speaking sat is defined as follows. One is given a set of N Boolean variables and a set of M constraints. Each constraint involves exactly three variables and is of the type variable number 1 is true or variable number 4 is false or variable number 5 is true.

The labels (from 1 to N) of the variables in each constraint are chosen randomly and each variable is required to be true or false by the constraint with probability one half. Surprisingly when the number N of variables and the number M of constraints go to infinity at fixed ratio

$$\alpha = M/N$$

there appears a phase transition at some critical value of  $\alpha$ ,  $\alpha_c = 4.26$ , such that when the ratio of constraints per variable is smaller than  $\alpha_c$  a randomly chosen set of constraints admits almost surely at least one solution while above this critical ratio there is almost never any solution.

This phase transition is interesting since it coincides with the instances which are the hardest to solve with existing algorithms, such as branch-and-cut procedures or local search algorithms. We have thus at our disposal a very easy way of generating seemingly hard problems!

Statistical physicists have studied this phase transition in detail in the past decade, and more generally the behaviour of the sat problem at any ratio. Here are a few results which were found:

- the value of the critical ratio locating the phase transition was calculated extending techniques invented by G. Parisi in the field of spin glasses at the beginning of the 80's. In addition another phase transition was discovered in the phase where solutions exist ( $\alpha < \alpha_c$ ). This phase transition corresponds to the clustering of solutions in groups of solutions far from each other in the variable configuration space. It has some deep consequence on the behaviour of local search algorithms.

- these physical techniques were in addition used to build a new algorithm to find solutions to random sat problems close to the phase transition. This algorithm, a new member of the family of message-passing algorithms (as Belief Propagation used in communication theory), finds a solution for ratios close to  $\alpha_c$  in average time polynomial in the number of variables, while from the worst-case point of view, sat is hard.

- the performances of classical algorithms, as branch-and-cut procedures, local search algorithms, has been characterized and understood to a large extent with statistical physics ideas and techniques. In particular the ideas of dynamical phase transitions, metastability, universality, have been shown to play an important role.

After one decade of intensive research and successes it is time to think about what is needed to go forward. As a first step it is certainly important to extend the above researches to less academic and more practical distributions of data. Distributions corresponding to industrial applications are available on large databases and existing algorithms are being tested upon those. Phase transitions are likely to take place, but the nature of the transition will be more complex than in academic, purely random distributions.

Another important direction is the understanding of finite size effects. Mathematical or physical theories are often based on the idea that "the size of the problem goes to infinity". While this assumption can give qualitatively excellent results, it never holds in practice and one needs to understand what happens for large albeit finite problems. Statistical physicists have answered this question for physical systems at thermodynamical equilibrium but what happens in dynamically evolving systems is far less understood.

On the long term the most important direction could be to understand in a better way how algorithms as message-passing procedures work and what tasks they can really achieve. The fundamental problem is to make work together many small processors located at the node of a network, with information flowing through the edges of those networks. While every processor is fed with local information (i.e. coming from its neighbours) the set of processors is capable of achieving a global task (i.e. to find a solution to the set of constraints). This kind of distributed architecture is ubiquitous in natural (biological) and artificial (e.g. the Internet) networks. The results obtained so far in the field of random optimization problems suggest that these algorithms are very powerful.

## **4.2 Networks, especially computer**

By Guido Caldarelli

One of the descriptions of complexity on which most of the scientists agree is that complexity arises when many independent parts of a system interact in such a way to produce a novel global behaviour. Put in this way, it becomes natural to think of network theory as one of the most natural tools in order to describe complex systems. Probably for this reason, the approach of complex network emerged spontaneously in different

areas and it now represents one of the few really interdisciplinary areas of research. Mathematically, all these systems used to be considered as haphazard sets of points and connections, mathematically in the random graph paradigm (Bollobás, 1985; Erdős and Rényi, 1960). This situation has radically changed in the last few years, during which the study of complex networks has received a boost from the ever-increasing availability of large data sets and the increasing computer power for storage and manipulation. In particular, mapping projects of the WWW (Adamic and Huberman, 2000) and the physical Internet (Faloutsos, Faloutsos and Faloutsos, 1999) represented the first chance to study the topology of large complex networks. Gradually, other maps followed describing many networks of practical interest in social science, critical infrastructures and biology. Researchers thus have started to have a systematic look at these large datasets, searching for hidden regularities and patterns that can be considered as manifestations of underlying laws governing the dynamics and evolution of these complex systems (Pastor-Satorras and Vespignani, 2004; Albert and Barabási, 2001).

Amongst the regularities that have been found we list the following:

- Many of these systems show the small-world property, which implies that in the network the average topological distance between the various nodes increases very slowly with the number of nodes (logarithmically or even slower) (Barrat and Weigt, 2000).
- A particularly important finding is the realization that many networks are characterized by the statistical abundance of "hubs"; i.e. nodes with a large number of connections to other elements. This feature has its mathematical roots in the observation that the number of elements with  $k$  links follows a power-law distribution, indicating the lack of any characteristic scale. This has allowed the identification of the class of scale-free networks which topological features turn out to be extremely relevant in assessing the physical properties of the system as a whole, such as its robustness to damages or vulnerability to malicious attacks (Caldarelli, Marchetti and Pietronero, 2000; Albert, Jeong and Barabási, 2001).

The attempt to model and understand the origin of the observed topological properties of real networks has led to a radical change of perspective, shifting the focus from static graphs, aiming to reproduce the structure of the network in a certain moment, to modeling network evolution. This new approach is the outcome of the realization that most complex networks are the result of a growth process. As a result, we currently view networks as dynamical systems that evolve through the subsequent addition and deletion of vertices and edges.

### Network Applications (so far)

The applications of network theory are several, here we restrict only on those related to computer science and biology, for which many progresses have been made. Different technological networks as the Internet (Faloutsos, Faloutsos and Faloutsos, 1999; Caldarelli, Marchetti and Pietronero, 2000) WWW (Adamic and Huberman, 2000), Wikipedia (Capocci et al., 2006) have been analysed with the tools of graph theory. One classical result is that the authority of a page on the web can be established by its PageRank (Brin, Page, Motwami and Winograd, 1998) that roughly corresponds to the probability for a random walker to visit it. This algorithm is at the basis of the search engine Google and triggered even more activity in the field. A particular important application can also be found in the field of cell biology. Both protein interaction and the interconnected series of reactions present in signaling have their natural description in the framework of complex networks. Apart from the obvious importance of these applications for medical science it has to be noticed that these two networks are interconnected, since complexes of interacting proteins can act as enzymes and develop a series of reactions that results in a signaling network. In this way we have one paradigmatic example of different networks related by a feedback. A similar situation

arises also in computer science where Internet and WWW are related by a similar relationship. Consequently theoretical progresses in the modeling of networks results in an increased understanding in both fields.

## Challenges

A key problem in the present society is the study of the formation and evolution of communities within the web and other social and technological systems. The knowledge of such communities is crucial to design better techniques for exploring those networks and retrieving specific information. As a particular case of social system can be considered those formed by financial institutions. In such a case a structure of complex networks with interconnected communities is at the base of lobbying in boards of directors (Battiston, Bonabeau and Weisbuch, 2003; Caldarelli and Catanzaro, 2004) and various correlations in stock prices and ownerships (Bonanno et al., 2005). Similarly the presence of communities in technological networks has also immediate and important meanings. The currently most successful strategy for web search relies on the Page Rank algorithm, which navigates the web by exploiting only its most basic link structure - how pages link to one another via hypertext links. But web documents (texts, images, media files and data) are also connected to each other by virtue of their membership in larger communities. Such communities - evident as clusters of densely interlinked pages -often have a thematic meaning based on some shared property. By focusing on the identification of such communities, we believe it will be possible to provide a thematic division of the web that will facilitate web crawling and information retrieval. Doing so will require an effective combination of the mathematics of graph theory and computer science with the traditional behavioural perspective of the social sciences, while also bringing in the modern techniques of statistical physics which are specifically suited for dealing with large systems such as the World Wide Web. Similar interdisciplinary efforts toward community characterization have already been successful in studies of the electronic communications infrastructure of large institutions. Communities are also the fingerprint of the presence of protein complexes (Gavin et al., 2002) and could play a great role in the identification of the development of signaling networks in the cell. The possibility to control such processes would have a series of immediate applications in medical science to cite only one example. Under this respect a "man on the moon" goal would be the mathematical characterization of complexity in the social, biological and technological structures.

## **5 COMPLEX SYSTEMS, BUSINESS AND SOCIETY**

By Stefano Battiston

The environment of business and government is obviously complex. But understanding their environment is not the only challenge of decision makers: they have to take decisions to deal with it and eventually to modify it. Fortunately, they did not have to wait until the 20th century and the emergence of complex systems science to adapt. In fact economics in the 18th century, operational research and management science in the mid 20th century, were born as answers to these challenges.

The strong increase in the complexity of our environment, the fastest rates of change, the necessity of delocalised and democratic decisions are now common wisdom. The limitations of standard approaches are related to the present situation: a strong increase in the complexity of our environment, a faster rate of change, the necessity of delocalised and democratic decisions.

- Standard approaches suppose full rationality and centralised decisions.
- They apply to independent or linearly dependant entities.
- The environment is static or supposed so.

The present situation clearly calls for a Complex Systems approach.

### ***5.1 Econophysics and Finance as a success story***

Finance became attractive to physicists because of the availability of large sets of financial data, which could remind them of the situation in physics where data are not a limiting factor. Financial time series were discussed and analysed by Mandelbrot et al. (1997), Mantegna and Stanley (1999), Bouchaud and Potters (2003) and the Santa Fe "school", Farmer (1999), Packard, etc. (which does not imply that economists did not also react). Any serious processing of these data yields results in contradiction with standard economics: e.g. fat tails in the distribution of returns imply non Gaussian statistics.

A number of physicists went into real finance: banks, brokerage and investment firms, and some even incorporate, creating successful start-up: Prediction Company in the US, Capital Fund Management in Europe, etc. Their successes based on techniques and concepts from complex system science concerned for instance portfolio management and foreign exchange markets.

These accomplishments were soon recognised by the academic community and by business, because they were fast and directly measurable as financial successes! Unfortunately the success of a long term policy in environment for instance is not so easily estimated.

Econophysics also brought new problems to the attention of academics, e.g. bubbles in financial markets, and new models, e.g. the minority game.

### ***5.2 Present challenges***

We shall now discuss, as examples, three domains in which CS offers significant contribution to economic and societal challenges:

- supply networks;
- credit and risk management;

- collective evaluation and trust-based networks.

The last part of this section will concern the barriers to the adoption of complex systems methods in the business and policy world.

### **5.3 Supply Networks Management**

A manufacturing system can be viewed as a network of buffers and machines through which several kinds of products flow. Ideally, the system should follow a stationary optimal regime. But, dependent on available information or forecasts, decisions need to be made which product is produced next on which machine. Even when simple heuristics are being used for making these decisions, the overall dynamics of a manufacturing system is complex and still not well understood. Variables of main interest are throughput (number of products produced per unit time), WIP (number of products in system), and cycle time (the time products stay in the system). Information and material flows in production and logistics systems suffer from a combination of the following characteristics: competition for scarce or expensive capacities, nonlinear effects and interactions, congestion, unpredictable dynamics, stochasticity, heterogeneity, local failures or breakdowns, network structures.

These features make the above systems highly complex, hard to describe, difficult to optimize, and almost impossible to control in real-time. This causes considerable inefficiencies in the use of hardware infrastructures as well as high investment and operation costs, which obstruct the implementation of new technologies. At the same time, an efficient use of new technologies is the key to competitiveness on a world-wide scale. The situation in the semiconductor industry is characteristic for the situation today: while there is steady progress in hardware technology, operational and logistic problems have been largely neglected. INTEL has identified the problem and invests into the optimization of their logistics, since an improvement by 3% only would save the company 1 billion US\$ each year. In order to make optimal use of newly available sensor, communication, and data processing technologies, one first has to gain an understanding of dynamic queuing networks and find ways to optimally control them. There are no suitable classical approaches to tackle this.

Classical approaches to production systems are based on Operational Research and Queuing Theory. These approaches have basically failed to describe the non-linear interactions between their various elements and the response to variations in demand. The fact that cycle times are large and non-linearly dependent on the load is one of the most difficult aspects in supply chain management; in particular as these systems suffer from inherent instabilities. Small variations of production parameters can generate a completely different dynamic behaviour. At certain critical parameter thresholds, one can observe discontinuous phase transitions from one dynamic behaviour to another one, including oscillatory patterns and chaos. The phase space of the system may even be fractal, which makes complex production systems particularly difficult to understand, to measure and control. Suitable modeling approaches have been formulated only very recently. Approximate, heuristic optimization methods such as genetic/evolutionary algorithms are too time-consuming as well. Instead, the optimization problems we face are more likely to be solved by decentralized control approaches in the spirit of collective or swarm intelligence. In principle, it is known that suitable local interaction rules can lead to coordination and optimization throughout the overall system. However, in contrast to systems close to equilibrium, there is no general theory for the evolution of stochastic, nonlinear, dynamic systems with network effects.

An example of a successful application of complex systems methods in this domain is the so called 'slower-faster' effect discovered by Helbing and collaborators. Their approach consists in modeling manufacturing processes as driven many-particle systems, where the discrete products and transport devices play the role of particles. For instance, the method was able to increase the throughput of a production chain in a major

semiconductor factory by up to 39%. In such a supply chain, silicon wafers, somehow similarly to photographic film, require a series of chemical processes. Treatment times can be shortened or prolonged only to a certain extent. The main problem in this system is the limited transport capacity of the handler, i.e. the device which has to move the wafers around. If several sets of wafers had to be moved at the same time, the treatment times for one of these would probably exceed the critical time threshold. Therefore, the challenge is to find a schedule that resolves conflicts. Interestingly, the problem of achieving coordination among several elements is similar to the coordination of pedestrians in the merging area in front of a door. The problem has been solved by the counterintuitive policy of increasing the treatment times. In fact with longer treatment times, the waiting times between successive runs are significantly decreased, resulting in higher throughput. That is, instead of stop-and-go patterns (waiting and usage periods of the chemical or water basins), a smoother output pattern was reached.

## **5.4 Credit networks and Systemic Risk**

Supply networks are subject to occasional production failures. Because supplier-customer relations often imply credit relations, production failures can also cause financial failures. The symmetrical causation, from credit to production failures, also exists. Due to the growing interdependence of supply and credit networks, both in terms of sector and geography, a natural question is do we predict and control the onset of failure cascades?

Quantitative study of risk is typically the realm of financial mathematics, but more recently also of physics (Bouchaud and Potters, 2003). The purpose of investigations is typically answering the question of how to minimize risk of individual firms or institutions, by optimizing a portfolio of actions. However, there is usually no concern for the so called systemic risk (Fecht and Gruener, 2005), the risk of collective damage in an economic system such as for instance the banking system, but also the network of suppliers and customers in a industry sector. One could expect that addressing this kind of questions with modern tools would be of concern of central banks since long ago. Surprisingly, even the UK central bank has started research on networks of banks only very recently (Yang, 2005).

In general, economic theory is not prepared to investigate avalanches in large heterogeneous networks. The common view on financial contagion is that connectivity is beneficial because it is a way of distributing risk. This is proven formally in some contexts: the optimal graph is found to be the fully connected one (Allen and Carletti, 2005).

However, in presence of a drift on the fragility, the opposite can occur. In fact, if each unit redistributes risk to the others, on one hand it delays its own default, but on the other hand the risk becomes very homogeneously distributed across units. If the general level of fragility increases, when eventually one unit defaults, all the others are very close to the threshold for defaulting themselves and a major collapse occurs (Battiston, Peters, Helbing and Schweitzer, 2006).

This kind of dynamics are suitable to be investigated with the methods of Complex Systems, capitalizing on the experience gained in the study on critical phenomena on systems such as sand pile and alike. However, it is important to stress the fact that economic systems have their own specificity and that theories cannot be simply transferred from sand pile to credit network. Brand new models have to be developed. Therefore future calls might emphasize that physicists have to team up with specialists of the discipline in order to develop models together.

An example of this desirable teaming up is the collaboration, in the study of systemic risk, of some researchers from the complex network fields with economists who have strong influence at policy design level in macro-economy (Battiston, Delli Gatti et al., 2006).

## **5.5 Collective Evaluation and Trust-based Networks**

### **5.5.1 Overview of emerging technologies**

We witness today a booming of new ways of marketing, trading and sharing information, which are made possible by a set of related emerging technologies. A first revolution occurred during the past century due to the availability of new techniques such as telephone, radio and especially TV. The present new wave is carried by the Internet.

Present day economic actors, firms and customers, can in principle retrieve a lot of information - in fact, most often, too much information to be usefully processed during the window of opportunity when decisions have to be taken.

Computerised information processing and data mining were developed as an answer to the information overflow, and the first commercial applications, such as customers' management, were used by firms. More recently, new applications were proposed to facilitate information retrieval and estimation of the quality of products and services to potential customers. These techniques are often based on the processing of information generated by customers who already acquired the product and tried it. They basically implement a reputation dynamics on computer; they also relate to more standard "ants algorithms".

Recommendation systems based on collaborative filtering suggest users items based on the similarity of their preferences to other users. For example, on amazon.com a user receives the message that "people who bought this book also bought these other books". This kind of recommendation systems works quite well for low-involvement items such as movies or alike. Many scientific teams are working on the data mining aspect, but the few works based on CS seem particularly promising (Laureti et al., 2002; Lauretti et al., 2006). The combination of collaborative filtering with trust is one the hot topics in computer science in the near future (Ziegler and Golbeck, 2006), and again the CS approach is proving to be quite successful (Battiston, Walter and Schweitzer, 2006; Walter, Battiston and Schweitzer, 2006). The fact that information is processed in a centralized way raises scalability problems. But more importantly, if ratings would concern high-involvement services, such as health care for instance, centralization raises also confidentiality issues. As we will see in the following, these limitations can be overcome with Trust-Based Networks.

The important aspect for complex systems science is that these technologies give rise to large-scale collective phenomena. While computer science research in this field focus either on the aspects of technological compatibility or security, the theoretical understanding of the large-scale emerging properties is poor. CS can and should give important contributions.

### **5.5.2 Potential Impact**

The emerging technologies around the concept of reputation, trust, collaborative filtering and P2P, make possible, for the first time in history, a large-scale real-time self-organization of citizens in completely new forms. For instance, these technologies make it easier for consumers to reach and share rating of products, independently of the producers. But it is also possible, for instance, that consumers form buying groups that negotiate with firms the delivery of products or services with specific features. Market diversity, which is today producer-driven, could become consumer-driven, a major change of perspective. In particular, the market share for sustainable products could increase significantly. The field of recommendation systems and akin does not reduce itself to targeted marketing. On the contrary, there is an unprecedented potential for empowering citizens to make more informed choices in their daily life in a vast range of domains, from purchases to political support. Some people even see it as a possible way of coping, not only with information overload, but also with stringent social dilemmas

such as those related to sustainable development. In fact, information overload and the tendency towards information monopolies interfere with today's EU Information Society commitment to preserve and manage the diversity of preferences and needs of citizens.

### 5.5.3 Trust-based Networks

Trust-Based Networks (TBN) can be defined as information processing systems in which interconnected agents (citizens, firms, organizations) share knowledge in their domains of interest. Each user has a list of buddies with which he decides to share lists of products, services, people, experts, etc., accompanied by his rating. Trust is built-on dynamically, based on the satisfaction experienced following the recommendations received from the buddies. Paths of high trust soon build up in the network, and each user is able to reach and rely on -filtered- information, even if coming from another user faraway in the network. This emerging property has some reminiscence to the building of optimal paths in ant algorithms. Some recent works have proved the overwhelming superiority of such trust based recommendation systems over those based on the frequency of the recommendations (Battiston, Walter and Schweitzer, 2006). From the point of view of scalability, TBN is naturally distributed and does not require centralized information.

There is no current established approach for investigating TBN. Some projects under IST deal with P2P networks, but here the CS approach is mandatory. Indeed, by means of a complex system approach, recent works have shown analytically that the performance of a TBN is robust within a wide range of crucial parameters such as link density among peers, heterogeneity of user preferences and sparsity of knowledge among users (Battiston, Walter and Schweitzer, 2006).

However, this is just the beginning of a quite dense research program. The main research objectives can be grouped as follows:

- Foundation from the perspective of Information and Network Theory:
  - small world properties to reach many domains of knowledge;
  - robustness against abuse and side-effects of herding and panic (e.g. decline of trust in health authorities due to food safety crisis around mad cow disease).
- Requirements of a distributed infrastructure supporting the TBN: performances, robustness, search engines;
- Design interaction mechanisms in order to:
  - encourage sharing and honest reporting;
  - discourage abuse and free-riding.
- Investigation of the social benefit of:
  - allowing users to assign different levels of privacy to their information (this has important applications in health-care and fields where confidentiality and management of sensitive data is a safety issue);
  - allowing the formation of coalitions, thus providing negotiation power on product/service features.

A TBN can be regarded as an IT support tool for decision making shaped around the natural behaviour of individuals in society. Today's search engines allow the user to find a range of information/products/services from a centralized source, corresponding to a set of keywords. Through a TBN instead, the citizen can search relevant items from specialized sources and evaluate the trustworthiness of the items with respects to her preferences.

In line with EU policy objectives (i2010), TBN empower citizens to make better-informed decisions on products and services, thus contributing to a competition based on quality. Not only consumers are concerned; also firms would be able to make more

informed choices on suppliers and partners. TBN can potentially increase the diffusion of knowledge as well as the transparency of products and services, with significant benefit for EU cultural development and economic competitiveness. It is hard to overestimate the benefit from such a system in terms of quality of life and satisfaction of citizens. TBN could be the future way in which interactions take place within sustainable societies and the EU has the chance to become the world wide leader and standard-setter in this initiative.

## ***5.6 Penetration of CS science in the business world***

Despite several success stories (some of which reported above), the penetration of CS science in the business world is still limited. Nonetheless, curiously enough, complex systems concepts are recognised at the corporate level.

An interesting evidence of this fact can be found in the report from annual IBM's Global Innovation Outlook (GIO), a forum organized by IBM, attended by around 250 leaders from business, academia, the public sector, NGOs and other influential constituents of the world community. The GIO takes a "deep look at some of the most pressing issues facing the world and works toward providing solutions to those needs". The report, which is worth reading, shows that the participants express themselves using concepts from CS science. Some are now relatively old, as self-organization, others are not originally from CS but have recently become prominent topics in CS, as social networks and supply networks. Finally, others are right now the subject of several on-going projects in CS, especially in the domain of ICT, as trust, reputation, collaborative environments. Very innovative visions have emerged from this forum of leaders, in particular regarding the future of enterprises and production networks.

But when it comes to applying complex systems solutions, recruiting personnel or consulting, the traditional perspective is still predominant. The issue is largely in the differences in language and culture between CS scientists and businessmen. Application of CS to business requires close collaboration and trust between the consultant and the customer. While traditional consultants and managers belong to the same culture (typically they both did an MBA in some business school), CS scientists have completely different language and mind setting. Consultant and managers are generally taught traditional approaches and are not competent in CS. It would be hard for consultants to educate themselves in CS, and even if they would do so, it would remain more difficult for them to sell CS solutions, compared to selling traditional ones. As a result, as long as they are able to make the customer believe that they are providing the best solution available, they do not have incentives in proposing CS-based solutions. It is hard to expect that business schools will teach managers to hire physicists to solve problems! The weight of culture and traditions might be lighter in Eastern Europe and indeed the success of start-up companies selling CS methods to business is encouraging.

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