Complex Systems

(Curator Eberhard Bodenschatz 11/16/2009)

Systems:

Systems are entities composed of well-defined components. When integrated the components act together as to form a functioning whole with dynamical behaviors and responses to the environment. Systems can be embedded into other functional entities as components. Identifying a system or a hierarchy of systems requires a certain level of abstraction and simplification. One delineates simple from complex systems.

Simple Systems have few components and their behavior is in all respects fully understandable and predictable. An example would be a solid ball falling under the action of gravity through air. This Simple System consists of the ball, the air, and the gravitational force. Here we usually assume a single ball, constant acceleration of gravity, a viscous drag on the ball, and Newton's laws. When making these assumptions, we arrive at very useful answers. We did, however, neglect many aspects. If, for example, we would ask how the behavior changes when we go from one ball, to two, to three, or even more balls that fall close to each other, our "Simple System" assumption fails. It is not sufficient to generalize from one ball's behavior to many. Instead we need to consider the interaction of the balls through their self-generated vortices. This makes the latter example a topic for Complex Systems Research.

Complex Systems may have many components (elements or spatio-temporal fields) that collaborate to create a functioning whole. Thereby the function creates itself, *i.e.,* it "comes about" by the dynamical interaction of the components without an intervening regulatory body. One speaks of "Self-Organization" or also of "Emergence". Important is that the word "complex" is not to be confused with the word "complicated". Let's consider, for example, an "architectural building complex" that serves a multitude of functionalities. As we all know it is not complicated, but shows its true functional complexity when we use it.

A well-known, simple example for a complex system where elements interact is a double pendulum that moves in the gravitational field [see the Science Express experiment]. While a single pendulum shows only two simple types of behavior -- swinging motion at low speeds and rotation in a fixed direction at high speeds, two coupled pendula show chaotic dynamics -- they switch in an apparently erratic manner between phases of rotation and of oscillations. Let's consider also another well-known example for a complex system where spatio-temporal fields like temperature, fluid velocity, and humidity collaborate, namely cloud patterns. They emerge all by themselves. All that is required is the thermal energy deposited by the Sun on Earth's surface, the heat radiated from the cloud top into space, the Earth's gravitational field, and the moist atmosphere. The dynamics and structure of the cloud patterns are sustained by the perpetual flux of energy from the Sun to the Earth and from the Earth's surface into space.

It is evident that Complex Systems span the whole spectrum from life sciences and medicine, physics, chemistry and engineering, to social, economic, and cognitive sciences. Research in Complex Systems requires a truly interdisciplinary approach that crosses traditional disciplines. In the following we will discus in detail further examples that include "Self-Organization and Pattern-Formation", "Complex Technical Systems", "Turbulence" and "Collective Phenomena". These examples only give a small glimpse of the field. Nevertheless they capture well the challenges and opportunities that lie ahead of us.

Complex Systems Research

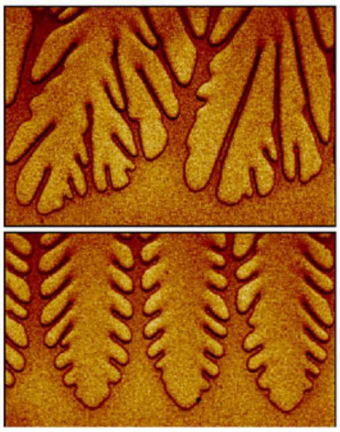
The key feature of complex systems is that the cooperative interactions of the individual components determine the emergent functionalities, which individually do not exist. Complex systems need energy to sustain their dynamical and structural behavior. Little changes in one component can have far reaching consequences for the system as a whole. Natural complex systems often show a high level of robustness due to redundancy in their components and interactions. Complex subsystems often combine to create new levels of functionalities. One of the main features of complex systems is that the behavior observed in different systems can be described by the same principles. For example, the aggregation of social amoebae [1], the catalytic gas reaction on a platinum surface [2] and the cardiac fibrillation that leads to sudden death [3] are all well described by the same theory.

It is the topic of Complex Systems Research to indentify and to understand the fundamental and general principles of complex systems. Theories need to be further developed that at the same time are sufficiently abstract and detailed as to apply to the wide range of classes of complex systems. They must capture the interaction of different temporal or spatial scales, the interplay between the individual history of a system and the universal features, the self-organized coordination of different elements or parts, the emergence of collective phenomena on the basis of local and nonlocal interactions, and so on. Complex systems research, therefore, encompasses the interaction between general principles and methods on the one hand and the detailed investigation of concrete complex systems on the other [4]. Identifying, understanding, and controlling the organizational, structural, and dynamical principles of complex systems and utilizing them for the benefit of human kind will be the challenge for the next decade and beyond.

Representative Examples:

(A) Self-Organization and Pattern-Formation:

The past two and a half decades have seen major progress in the theory of pattern-forming, self-organizing systems. An example of a pattern-forming process that determines the material properties of metallic alloys, as used in turbine plates of airplanes, is given in Fig. 1.



- Figure 1: Dendritic single crystal growth of a model alloy between two plates in a temperature gradient. The selected solidification pattern depends on the direction of the growth with respect to the crystalline axes [5]. Dendritic structures like these determine the mechanical properties of super alloy turbine plates and of metallic alloy casts. In single crystal growth for semiconductor technology instabilities like the one shown need to be avoided.

Numerical simulation and advanced experimental tools now allow highly resolved quantitative investigations of the spatio-temporal evolution, not only of spatially extended systems [6], but also of highly coupled networks. This is well illustrated by the example of epidemic outbreaks and the subsequent geographic spreading of the infectious disease. For diseases that are transmitted from person-to-person, the spreading is caused by human mobility. Pathogens can be transported by air travel and generate new nuclei of infection on long distances. The resulting patterns rather resemble a fractal than a spreading front. In a recent empirical and theoretical study this statistics has been explored irrespective of the means of transportation by using banknotes as a proxy [7].

Concurrently to Physics, Chemistry and Material Science, Biology and Medicine are progressing rapidly. We are gathering an ever-increasing amount of quantitative data. In the life science this includes patterns of gene expression and protein interaction in time and space during biological function and development. New imaging technologies (high speed imaging, nano-scale fluorescent imaging of proteins, ultrashort x-ray imaging, cryo-electron microscopy etc.) give us fundamental data into the complexity and pattern formation from the molecular and intracellular scale, to the multi-cellular scale of whole organs and organisms. Experimental tools begin to interface with, manipulate, and control the dynamics of biological cells with a spatiotemporal precision that matches the microscopic organization. For example, on the level of single neurons, in vitro fast multi-site uncaging of neurotransmitter applied to dendritic arbors can mimic the complex distributed patterns of synaptic inputs received in vivo. Genetically encoded light-gated ion channels and pumps now allow the control of precise temporal patterning of ion channels.

These emerging techniques are driving a revolutionary change. This allows for the first time to quantitatively address many long-standing questions about the mechanisms of pattern-formation and self-organization from Physics, Chemistry and Material Science, to Biology and Medicine. Progress requires seamless collaboration across all disciplines and with it a new breed of scientists that are knowledgeable both in the field of complex systems and their specific field of scholarship.

1. Complexity of Heart and Mind

Among the organs of our body, the function of heart and brain are unique in that their operation emerges from the collective dynamics of millions of strongly interacting cells well organized in their geometrical structure and connectivity. In the heart muscle the propagation of a nonlinear wave pulse, the cardiac action potential, controls the contraction. Usually the propagation is well organized both in space and time and the heart functions as an efficient biological pump. During cardiac fibrillation, synchronous contraction is disrupted by vortex-like rotating waves of electrical activity resulting in spatio-temporal-chaotic excitation patterns (see Fig. 3) [3].

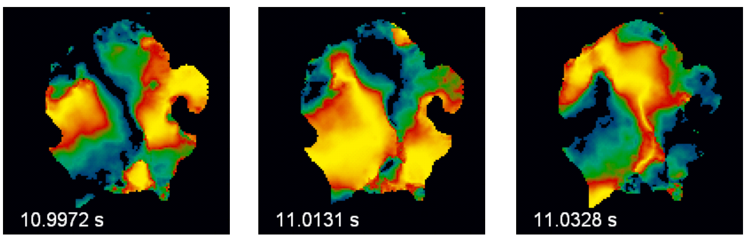


Fig. 3: Cardiac fibrillation: spatial-temporal chaotic electric excitation pattern on the surface of heart tissue (field of view 6 x 6 cm^2). Colour code: black = resting tissue, yellow = excited tissue. The missing synchronization leads to the failure of the heart as a pump and to sudden death.

This electro-mechanical malfunction of the heart can rapidly evolve into Sudden Cardiac Death, which causes an estimated 738.000 deaths per year in the European Community alone. Yet the physical mechanisms underlying the dynamics and control continue to pose a fundamental scientific riddle.

Similarly, in the brain the propagation of a nonlinear wave pulse, namely the neural action potential, is at the basis of the computational and memory power of the brain, *i.e.,* what determines the workings of our 'minds'. Here, however, due to the high degree of interconnectivity and topological complexity of the neuronal network, the coordinated activity of millions of interacting nerve cells is more complex. The field of network dynamical systems is largely driven by the steady stream of novel dynamical phenomena that result from the interplay of local nonlinear dynamics and complex network structure. Also, the real time processing of input interacts with the slower process of learning through activity dependent changes of synaptic weights [8,9]. The brain, however, would be only incompletely understood when just viewed as a complex dynamical system. For example, the processing of hierarchically structured sequences (sentences) can be described at the neural systems level as an input driven initial phase of local structure building which is immediately followed by a second phase of building hierarchical dependencies [31]. This specific ability to extract rules underlying hierarchical dependencies appears to differentiate humans from non-human primates. Therefore, understanding the operation of the mind also requires describing and analyzing its emergent information processing functions. To achieve this, many aspects of neural computation have been successfully formulated as problems of pattern-formation, statistical inference and optimal decision-making, phrasing them in the mathematical language of statistical physics [10-12].

Key questions:
On the network level:

- Can one achieve effective control of a network state by control or inactivation of a structurally defined subsystem?
- What information is emerging from projects that define anatomy first at the level of pathways and later at the level of individual connections?

At the systems level:

- Can one use the intrinsic plasticity of neuronal processing architectures to reprogram functional connectivity with spatiotemporally structured neurostimulation?
- How can we use the approaching ability to open and restore brain feedback loops to make progress in understanding the algorithms of sensorimotor control? How can we reproduce these algorithms to develop functional neural prostheses?
- How can we control malfunctioning pattern-formation with application to cardiac arrhythmias, migraines, and epilepsy?
- What features are generic and which ones are specific? How can they be captured in theoretical models?
- How can genetic mutations and gene manipulations be used to guide the self-organizing behavior.
- Is sensory input during brain development sufficient for the growth of higher cognitive systems (such as comprehension, reasoning, decision making) or is it a necessary condition to trigger a biologically determined system?

Outcome and Benefit:
This advanced dynamical understanding of complex biological systems and their dependence on genetic and environmental factors, will open – on a long-term perspective – new paths for translating fundamental scientific discoveries into practical applications that may improve human health. Neurobiological systems will also, at a very fundamental level, inspire new artificial schemes for the processing of large and complex data sets.

2. Cellular organization of life: from intracellular dynamics to the emergence of patterns and shapes.

Higher organisms develop by the collective organization of many cells. These cells multiply by repeated divisions and create widely varying morphologies. The biological cells themselves are complex systems that utilize highly evolved genetic regulatory schemes to create structures that can dynamically maintain themselves or contribute to a higher multi-cellular organism. These regulatory schemes in turn integrate complementary types of information, the internally stored genetic and epigenetic one and the externally provided and variable information from the environment or other cells via specific signals [13]. On the single cell as well as the multi-cellular level it remains a fundamental challenge to understand the principles underlying the developmental process that lead to the formation of complex patterns and morphologies. The collective behaviors of many cells are guided by their physical properties and active behaviors. Approaches from statistical physics and soft matter physics play therefore an increasing role for the understanding of multi-cellular systems. An example of current study is the two-dimensional tissue, the so-called epithela. Physical descriptions of the dynamics of cell packing reveal that the tissue as a whole behaves as an active form of matter, being dynamically remodeled and exhibiting dynamic behaviors as a result of cell division and cell death. [14-17]

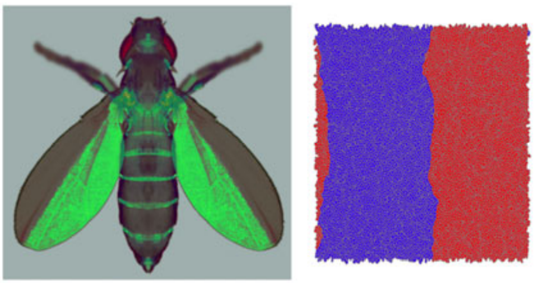


Figure 3: Tissues are organized in cellular compartments separated by sharp interfaces. In the fly wing two compartments are apparent by a GFP labeling of cells (left, courtesy of Christian Dahmann). Simulation of a compartment boundary generated by increased cell bond tension (right, courtesy of Frank Jülicher)

The combination of cellular signaling for example by morphogens with cell division and cell flows suggests that novel mechanisms for pattern-formation are at work. A key process is the control of the cell division axis, which determines cell rearrangements and its emergent behavior.

Key questions:

- How can the knowledge about cellular signaling and information processing be combined with cell material properties, adhesion control, chemotaxis, mechanotaxis, and other active behaviors?
- How can mutations and genetic perturbations be used to study the effects of altered properties of cells and their signaling activity?
- How do many cells organize their growth to a well-defined size and shape?
- How is the decision to divide cells taken collectively and implemented by local rules?

Outcome and Benefit:
The combination of quantitative experiments with theory is expected to permit the characterization of fundamental mechanisms underlying cellular organization into functional biological matter. Long-term challenges are to understand dynamic organization in three dimensions, to get insights of how macroscopic morphologies are encoded in the genome. This will clarify how the developmental process is robust in the presence of fluctuations and variability.

(B) Complex Technical Systems

In the past significant progress has been made to increase the productivity, selectivity, and sustainability of chemical and biotechnological production processes. But in the next two decades, further scientific and technological breakthroughs in process systems engineering are needed in order to organize the transition from fossil fuels and petro-chemical feed stocks towards renewable energies and raw materials, thereby closing CO_2 cycles by integrating biological substances. To accomplish this challenging task, theoretical and experimental approaches need to be developed for the analysis and design of chemical and biochemical production systems with focus on their inherent multi-level structure.

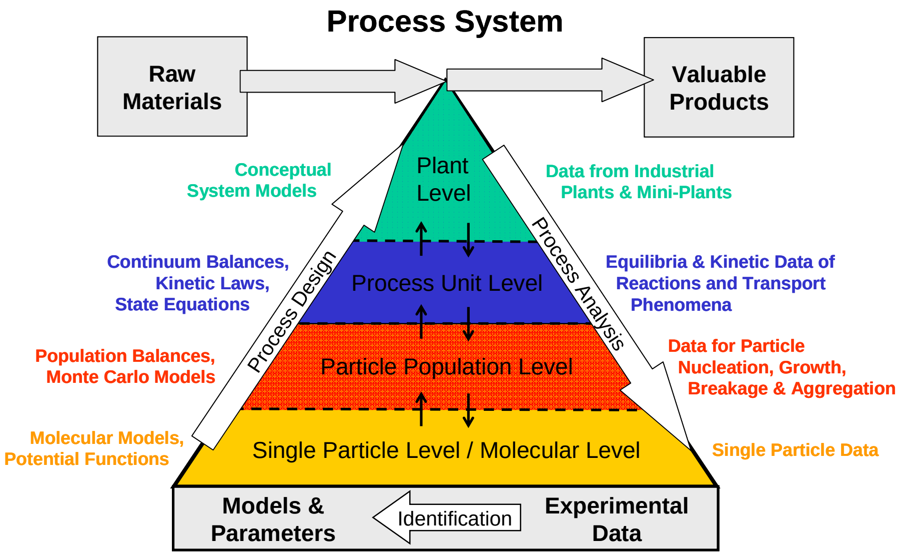


Figure 4: Multilevel structure of chemical and biochemical process systems. (courtesy of Kai Sundmacher)

As illustrated in Figure 4, the plant level of each production process can be decomposed into process units, each consisting of a number of interacting thermo-dynamic phases. Each phase can be represented as a distributed particle population, *i.e.*, an ensemble of interacting single particles such as cells, crystals, bubbles etc. or single molecules. In regards to this multi-level structure, process analysis is a top-down procedure, dealing with the modular decomposition of larger entities into smaller units, while process design is a bottom-up task, aiming at the aggregation of functional modules from lower to upper levels in order to generate a complete production system.

Key questions:

- How should we organize flows of mass, energy and information in chemical and biochemical production processes to achieve highest efficiency and selectivity? [18]
- How can we understand the organizational principles and behaviors of cellular systems, e.g. adaptivity and robustness [19] and how can we make use of them in designing efficient biotechnological processes? [20]
- How can we hierarchically control complex production processes from the level of individual particles up to the plant level? [21]
- How can we control multiple operating states, which can emerge from the nonlinear properties of complex chemical processes? [22]
- How can we design dynamic stimuli to drastically enhance the performance of technical processes and systems? [23]
- What are the best strategies in formulating reduced mathematical models that still reflect the essential dynamics of large-scale systems, as a prerequisite for process control? [24]

Outcome and Benefit:
New technological and production processes based on complex systems research promises to close CO_2 cycles, enhance efficiency of production processes, and to incorporate biological substances and function in new materials and products.

(C) Turbulence

Turbulence manifests itself in myriad ways across the physical, chemical, engineering and even biological sciences. It occurs whenever fluid viscous forces are small compared to the dominant driving forces of the flow; in practice this includes most macroscopic natural and technological flows. The mixing and transport properties critically impact the fundamental behavior of phenomena found in astrophysics, in fusion and plasma physics, in earth, solar and planetary sciences, in process engineering, and in the ecological sciences [25]. Turbulence is a fundamental topic in fluid and dynamical systems research and among others, raises basic questions in both applied mathematics and informatics. The subject of turbulence unites students of the terrestrial biosphere studying the exchange of heat, momentum and matter within the forest canopy, with physicists exploring strategies for confining plasmas, with mathematicians developing fundamental theories and numerical methods, or computational scientists designing methods for structuring computations across hundreds of thousands of computational elements.

Key challenges:

- Turbulence is key to the spread of pollutants, aerosols and bio-agents in the biosphere. Unclear is how turbulence influences particle dynamics as function of particle density, size, and concentration, and how particles at higher concentration affect the dynamics of the flow [26].
- The lack of understanding of the coupled turbulence/aerosol dynamics and of convective currents underlies a persistent uncertainty in the prediction of the earth's future climate. A better understanding is needed to evaluate pressures on environment and climate from anthropogenic and natural emissions and to render more precise the predictions on the energy balance due to phase changes that are highly coupled to the dynamics of drop formation in turbulent clouds and the concomitant effect on radiation balance [27].
- The transfer of energy due to thermal convection determines the structure of planets and stars. A better understanding of high Rayleigh-number turbulent convection and of turbulent boundary layers is needed.
- In wind energy gain is maximal for the highest wind speeds, i.e., strongest turbulence. Current technology does not incorporate well the effect of turbulent velocity fluctuations on the design of wind-turbines. A better knowledge of turbulence and its interaction with wind-farms at the large scale and the propeller turbulence boundary layer interaction at the small scale is needed to advance the technology.
- The future of fusion reactors relies on an efficient confinement of the plasma. Instabilities and turbulence disturb this confinement. A better understanding of turbulence and its control is needed to bring fusion from the laboratory to the power plant.
- The development of more efficient and environmentally friendly air, ground, and water transportation relies to a large part on the development of quieter, cleaner and more efficient propulsion systems. Progress requires a better knowledge of turbulent fluid flows in turbines and engines.
- Any process of energy efficient combustion and burning requires turbulent mixing of the combustibles. Better fundamental stochastic models for turbulent mixing are needed to allow for the development of more efficient and cleaner technologies.
- Turbulence determines the environment of plankton, which is the main food source for most higher developed ocean life. Currently, our understanding of the effects of turbulence on the biology of plankton is rudimentary.

- Transport of aerosols and sand plays an important part in erosion and desertification of land and forest environments. An increased understanding of the impact of turbulence in boundary layers and aerosol transport is needed for better management and risk assessment of biological resources.

- The clustering of matter in the beginning universe, as well as the initial stages of planet formation [28] is attributed to turbulence. Detailed mechanisms although proposed are not clear due to a lack of knowledge of particle transport in turbulence.

Outcome and Benefit:
An increased understanding of turbulence promises huge advances in science and technology. Be it the Earth's climate, energy generation, transport, oceanography or astrophysics a better knowledge and mathematical description of turbulence will rake huge benefits.

(D) Collective Phenomena far from Eqiluibrium

A particularly well-defined and easily accessible model system for the study of collective phenomena far from thermal equilibrium is a granular gas. In the recent past, it has been shown that phase transitions in wet granular gases can be well understood on the basis of just a few characteristic parameters [29]. This demonstrates similarities with the universality in equilibrium phase transitions, although in the case of a granular system, large granular temperature gradients are present in steady state. In simulations of driven dense granular gases a Kolmogorov-type instability accompanied by periodic undulations and, at stronger drive, chaotic behavior has been observed [30] suggesting similarities between granular gases and fluids.

Key questions:
- Is a granular gas behaving as a isothermal fluid?
- Is it possible to identify similarities between equilibrium states and non-equilibrium steady states and understand under which circumstances and in what respect these types of systems can be mapped upon each other?

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