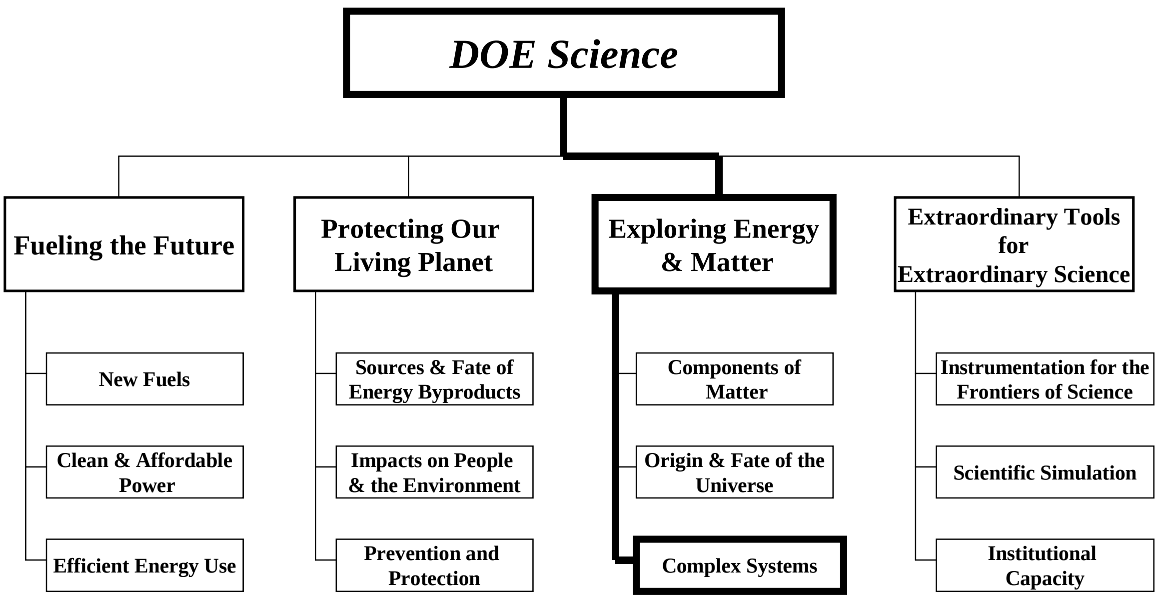
Chapter 10
Complex Systems

Scientific Challenge: ***To understand and control complex systems of matter, energy, and life.***



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Much of the research of the past 50 years has been devoted to solving very difficult problems in idealized, simple systems. The challenge now is to use that knowledge to better understand complex systems involving collective phenomena and adaptive systems.

Radically different, complex systems appear when many entities come together, interact or adapt. Complexity in natural systems typically arises from the collective effect of a very large number of components. At present, it is often impossible to predict the detailed behavior of any single system's component, or, in fact, the precise behavior of the complete system. But the system as a whole may nevertheless show definite overall behavior, and this behavior usually has several important features. A wide variety of systems exhibit overall behavior. For example, the many aspects of magnetic phenomena, ferromagnetism, anti-ferromagnetism, and spin waves are attributable to the collective behavior of many spins; and the ability to think and adapt to surroundings is the result of complex behavior of many neurons.

The time is ripe for further emphasis in understanding complex systems because of new theoretical and experimental methods and results. For example, third generation synchrotrons allow measurement of weak signals and determination of structures of complicated molecules and materials. We can now study interfacial phenomena directly using intense x-ray beams. Increases in computational power make it possible to do realistic simulations of non-ideal systems in reasonable times. New synthesis techniques, such as combinatorial chemistry, make it possible to synthesize large numbers of compounds very quickly to search for combinations with certain properties and to test and refine theory. Combined, these techniques are creating an opportunity to bridge the gap in understanding between atomic and molecular properties and the bulk structural and mechanical properties of materials. and to create new, better materials.

Whole genome sequencing and analysis are providing a new paradigm for biological research. The ability to determine the complete genetic potential of an organism permits a context for integrating individual molecular, biophysical, biochemical, cellular and physiological processes and events into a fuller understanding of living systems. The understanding of biological systems at ever-increasing levels of complexity promises to usher in a new age in biological research.

Collective Phenomena

Description, Objectives, and Research Performers

The challenge at the frontiers of basic research is to obtain fundamental understanding of increasingly complex systems. Systems composed of many elements show some unique behavior patterns, which may be called "collective phenomena." Recent progress in science sheds new light on these complex phenomena. Classical physics considers systems of particles; now, more sophisticated elements are coming within our scope of study. For example, scientists are systematically analyzing fundamental paradigms of collective phenomena; relevant research is being conducted on the physics of nonlinear waves (solitons), fluid dynamics, plasma physics, spectral theories, phase transitions, turbulence, and self-organization in complex systems. Such research involves multidisciplinary and interdisciplinary efforts and holds the promise of delivering revolutionary breakthroughs. It bridges the gap between an atomic level understanding (reductionist view) and a continuum mechanics understanding (classical view) of complex and collective phenomena. Research is conducted predominantly at national laboratories and universities.

Research Challenges and Opportunities

Important areas of inquiry in the field of collective phenomena include the following: (1) Classes of non-equilibrium materials that will be key elements of the next generation of energy technologies pose new challenges and opportunities because of their complexity. (2) Despite their importance, catalytic processes are not sufficiently well understood to allow for the rational design of new catalysts. Models for catalytic action are limited in scope and applicability. (3) Even though photosynthesis has been studied for decades, we still do not completely understand it nor have we been able to duplicate or improve on it. This one example of the control of entropy — the ability to mimic the functions of plants — remains one of the outstanding challenges in the natural sciences. (4) A major unsolved problem is the physical mechanism that makes high-temperature superconductivity possible. (5) A challenging issue is giant or colossal magnetoresistance. (6) We understand single atoms, molecules, and pure crystals fairly well; but, when we go beyond these simple systems to larger more complex systems, our understanding is limited. Understanding phenomena over wide timescales is also important — from femtoseconds in spectroscopy, to decades in the regulatory system of plants, to thousands of years in radioactive waste disposal.

Research Activities

Office of Science-sponsored research spans the materials, chemical, plasma, geological, engineering, geological plant and microbial sciences. Research in chemistry, materials, geosciences, and biosciences covers lengths from the atomic scale to the cellular scale to the meter scale and times from femtoseconds to millennia. For example, theory and simulation of plasma behavior in both magnetic and inertial fusion is complex because of the many orders of magnitude in spatial and temporal scales involved. Examples of research into collective phenomena include non-equilibrium systems, functional synthesis, control of entropy, strongly coupled systems, and heterogeneous systems.

Non-equilibrium systems. Areas under investigation include high-temperature superconductors, which are complex compounds of four or more elements that are not stoichiometric with respect to oxygen; and the glassy metal state, which has many desirable properties, but no long range order or symmetry. Researchers are discovering that many interesting and useful properties exist in atomic and molecular arrangements that have minimal dimensions, such as those found in thin films, membranes, and quantum dots. Other examples include polymers, molecular magnets, biomolecular materials, and new inorganic materials, all of which are important in applications such as fuel cells, batteries, membranes, catalysis, electrochemistry, and photoabsorption. A very exciting area of research is in biomolecular materials. Biological models are being used to make better polymers; to develop self-assembled, three-dimensional structures; to make very sensitive sensors, and to deposit hard inorganic coatings.

Functional synthesis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes.

The control of entropy. Photochemistry research investigates, at the molecular level, fundamental processes that capture and convert solar energy. This research encompasses organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry. Naturally occurring photosynthetic reaction centers and antenna systems are studied as models of biomimetic/photocatalytic assemblies that can carry out efficient photoinduced charge separation.

All living systems control entropy. Basic research on plants includes photosynthetic mechanisms and bioenergetics in algae, higher plants, and photosynthetic bacteria; control mechanisms that regulate plant growth and development; fundamental aspects of gene structure, function, and expression; plant cell wall structure, function and synthesis; and mechanisms of transport across membranes. Research in these areas seeks to define and understand the biological mechanisms that effectively transduce light energy into chemical energy, to identify the biochemical pathways and genetic regulatory mechanisms that can lead the efficient biosynthesis of potential fuels and petroleum-replacing compounds, and to elucidate the capacity of plants to remediate contaminated environments by transporting and detoxifying toxic substances.

The research focus in the microbiological sciences includes the degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of microbial growth and development, thermophily, e.g., bacterial growth under high temperature, and other phenomena with the potential to impact biological energy production, conversion and conservation. Organisms and processes that offer unique possibilities for research at the interface of biology and the physical, earth and engineering sciences also need to be studied.

Strongly coupled systems. Research aimed at a fundamental understanding of the behavior of materials includes experimental measurements to determine electronic structure, transport properties, phase transitions, mechanisms for high temperature superconductivity, complexity in electronic interactions, self-organization of electronic states. The materials examined include magnetic materials, superconductors, semiconductors and photovoltaics, liquid metals and alloys, and complex fluids. The measurements include optical and laser spectroscopy, photoemission spectroscopy, electrical and thermal transport, thermodynamic and phase transition measurements, nuclear magnetic resonance, and scanning-tunneling and atomic-force microscopies. The development of new techniques and instruments including magnetic force microscopy, electron microscopic techniques, and innovative applications of laser spectroscopy are necessary to understand coupled systems.

Fusion involves complex coupling of particles and fields. Although there has been marked progress in understanding macroscopic equilibrium/stability and turbulence and the associated transport in plasmas, improved theories and simulations are needed to quantitatively predict the behavior of fusion plasmas. Current models of equilibrium and stability must be extended to be fully three-dimensional and to include fluid and kinetic effects. Simulations of ion turbulence and transport should be extended to include electromagnetic effects and improved models of electron dynamics. In addition, new approaches to understanding energy transport in tokamaks, such as Self-Organized Criticality, are being investigated to understand their applications to fusion plasmas. Ultimately, integrated models, capable of complete simulation of both magnetic and inertial confinement systems, must be developed.

Heterogeneous systems. New research involving advanced computational and experimental approaches for treating complex mineral-fluid interactions will improve the understanding of fundamental processes and their interactions over a wide range of space and time scales needed for quantitative predictions of the consequences of transport and use of energy and material within the Earth's crust.

Accomplishments

- Proof of a thermodynamic first-order transition from a solid-like vortex lattice to a vortex liquid in a high temperature superconductor is leading to development of a new state of matter called vortex matter. The nature of the transition is significant for fundamental theories of phase transitions and also for practical applications of superconductivity.

- A metal-insulator transition has unexpectedly appeared in a MOSFET (Metal-oxide-semiconductor- field-effect-transistor) subject to strong electric fields at low temperatures. This is remarkable, because a MOSFET operates as an ultrathin sheet of electrons on the surface of the silicon semiconductor and, according to established theory, should not conduct at very low temperatures. This behavior is very consistent with what is observed for other superconductors, and the observation has sparked considerable interest in the scientific community.

- Pencil-shaped organic molecules called "rod-coils," designed and synthesized to have half of the molecule rigid and the other half flexible, were discovered to exhibit unusual and important clustering mechanisms on several size scales. Because the building-block molecules are all oriented in the same direction, the film’s properties mirror those of the individual molecules, resulting in a film whose bottom surface is sticky and top surface is slippery. Such a film has many potential applications, for example, as an anti-ice coating on an airplane wing or an anti-blood-clot lining for artificial blood vessels.

- An atom-tracking STM was developed for direct measurement of surface dynamics.

- Magneto-optical imaging of magnetic vortices and transport currents in superconductors were accomplished.

- First principles quantum simulations of atomic structure, electronic conductance and dynamical fluctuations in metallic nanowires and carbon nanotubes have been performed. The results of these investigations allow deep insights into the physical nature of low dimensional materials systems and provide impetus for laboratory experiments aimed at the development of nanoscale devices and atomic scale switches.

- Prediction of multilayered semiconducting materials led to the production of a 30% efficient photovoltaic device now used in outer space.

- Recent three-dimensional simulations of turbulence, transport, and macroscopic stability in fusion plasmas have provided insight into the fundamental processes at work. For example, three-dimensional turbulence simulations have shown that zonal flows can lead to the formation of "transport barriers" in plasmas, thus dramatically reducing the loss of energy and particles.

- Understanding the physical mechanism responsible for high temperature superconductivity remains the outstanding problem in modern condensed matter physics. Recent experiments and theory indicate that, unlike common metals, electric currents in these superconductors are like rivers of charge, separated by atomic magnets present in the system. The picture resembles the stripes on a flag, which can be static or dynamic like a flag waving in the wind. Theory has shown that the interaction between the rivers of charge and the atomic magnets may be the key to understanding the exotic superconductivity in these materials.

- Traditionally, catalytic science has operated in two separate regimes: in solution (homogeneous), and on surfaces (heterogeneous). Each type of catalyst offers its own distinct advantages, but until recently attempts to interface the two centered on the use of easily studied homogeneous molecular catalysts to model putatively analogous phenomena on surfaces. Recently, has taken the opposite tack—attaching molecular catalysts to surfaces and exploiting the unique properties of each. This resulted in unique synergism, creating interesting new catalysts whose properties can be controlled through variations in the molecular catalyst and the supporting material. This new catalysis has the promise of creating new catalytic materials and generating fundamental knowledge that will result in a better understanding of catalytic phenomena.

- A combinatorial chemistry system has been devised for optimizing physical and chemical properties in which the chemical composition of a material can be changed, with each composition located at a point on a grid. The performance of each composition is then tested and the optimized composition can be selected easily and rapidly. Combinatorial chemistry is one of the important new methodologies to reduce the time and costs associated with producing effective, marketable, and competitive new substances. Scientists use combinatorial chemistry to create large populations of molecules, or libraries, that can be screened efficiently en masse. The field represents a convergence of chemistry and biology, made possible by fundamental advances in miniaturization, robotics, and receptor development.

- Techniques were developed to synthesize nanocrystals and to assemble them into useful structures. For example, a spray specialized atomization process produced a novel nanocrystalline composite powder with a crystallite size that matches that of a magnetic alloy. Adding the nanocrystals to the alloy produced stronger and cheaper high-strength, permanent magnets. The permanent magnet industry was worth $3.2 billion globally in 1995 and is predicted to reach $10 billion by 2010.

Adaptive Systems

Description, Objectives, and Research Performers

Research on complex, adaptive systems is the study of the behavior of macroscopic collections of individual units that are endowed with the potential to evolve in time. Their interactions lead to coherent behavior that can be described only at higher levels than those of the individual units. Hence, the whole is more than the sum of its components. For example, life forms survive by adapting to change. They evolve successfully or perish. These complex, self-organizing systems are adaptive, in that they don't just passively respond to events. Common underlying organizing principles are at work; these are the concern of fundamental studies in complexity. Two major research areas are concerned with understanding gene function and ecological processes. The research in these areas is conducted at national laboratories, universities and industrial firms.

Research on gene function provides information needed to understand the structure and function of the proteins and RNAs encoded by the human (and other) genome and to understand the nature of the regulatory networks that control expression of multiple genes in space and time. This information is fundamental to our understanding of the human genome and the genomes of microbes with broad applications in energy, the environment, medicine, agriculture, and industry.

Research on ecological processes advances scientific understanding of responses of terrestrial ecosystems and organisms to changes in climate and atmospheric composition, such as alterations in temperature and moisture and increases in carbon dioxide concentration. Objectives are to improve understanding of (1) the responses of terrestrial organisms and ecosystems to simultaneous changes in atmospheric composition and climate; (2) the causal mechanism or pathway of the responses and the biological and ecological processes controlling the responses; and (3) the extent to which the responses are manifested across different organizational (hierarchical) levels of terrestrial ecosystem components and processes of value to humans.

Research Challenges and Opportunities

Even the most primitive living organism controls the structure and function of its diverse products far better than the cleverest chemist. Understanding the structure, function, and regulation of genes at a genomic scale will be one of the great challenges in biology for the next several decades. In the past, questions of gene structure, function, and regulation have generally been addressed one gene at a time. With the availability, in the next several years, of sequence information for the entire human genome and for the genomes of many simple and complex organisms, this one-at-a-time approach will not keep pace with the availability of information on human genes. The national capabilities in genomics, structural biology, instrumentation and automation development, and the use of model organisms, such as the mouse, can be used to make important contributions to this new field of biology.

Knowledge of possible effects of climate and atmospheric changes on ecological systems has increased over the past decade and qualitative estimates of responses to such changes can be developed. However, our current ability to make quantitative predictions of the effects of alterations in climate and atmospheric composition, such as increasing atmospheric carbon dioxide levels, on any particular ecosystem at any particular location is constrained by a limited understanding of many critical processes. Furthermore, the structure and functioning of terrestrial ecosystems are influenced by multiple climatic and non-climatic factors, the interactions of which are not always linear or additive. Further, very little research has studied the dynamic responses of ecosystems to simultaneous changes in multiple factors, particularly human-induced environmental changes to which ecosystems have not been previously subjected.

Research Activities

Research capitalizes on our understanding and the manipulability of the genomes of model organisms, including, for example, yeast, nematode, fruit fly, Zebra fish, and mouse, to speed understanding of human genome organization, regulation, and function. An important goal is to develop and use experimental systems and resources to characterize or analyze human gene function that match the speed of new gene discovery on a genomic scale. Research will closely coordinate with structural biology research that will develop high throughput technologies to provide information on gene structure.

Experimental and modeling studies on different types of ecosystems to investigate system responses to alterations in climate variables, atmospheric CO_2, ozone, and nutrient inputs. Studies using the Free-Air CO_2 Exposure (FACE) technology investigates the response of different types of ecosystems, including forest, grassland, desert, and croplands to elevated CO_2 and other environmental changes. A Throughfall Displacement Experiment is an experimental study of the response of a forest ecosystem to changing precipitation inputs. These experiments document responses to the experimental treatments, including the range of adjustments in physiological processes, above and below ground growth responses, and other structural and functional responses of the treated and reference or control ecosystems being studied. Results will be used to parameterize and test ecosystem response models that will be used to assess the consequences of human-induced environmental changes on terrestrial ecosystems.

Accomplishments

- Critical contributions in gene research include the development and application of flow cytometry, cDNA arrays, bio-chips for the parallel analysis of genes or proteins, algorithms to identify putative genes, strategies to induce and analyze mouse mutants, demonstration of gene regulatory mechanisms in DNA, cells and tissues, and tools and strategies for studying and characterizing human gene function in large blocks of DNA or fragments of chromosomes.

- Initial results of 7 long-term experiments on physiological and growth responses of forest, grassland and crop species and ecosystems show that increased CO_2 caused greater productivity and improved water use efficiency of these systems. A significant part of the productivity increase occurs below ground with roots, soil micro flora and the formation of soil organic matter.

- Findings from the Throughfall Displacement Experiment after six years show that changes in the seasonal timing of rainfall has a greater effect on the productivity of forest ecosystems and carbon sequestration by forests than a uniform change in rainfall applied throughout the year.

Portfolio Summary

This portfolio area, “Complex Systems,” encompasses research from many programs and supporting activities that crosscut the research topics covered above. The table below summarizes specific core research activitiesthat strongly support or moderately support Complex Systems, including collective phenomena and adaptive systems. The funding totals for these areas are an analytic tool reflecting the highly crosscutting, leveraged aspects and implications for individual research areas within DOE’s science portfolio. **Because research areas may appear in multiple chapters, there will be significant instances of multiple counting, and the chapter totals will not sum to the overall science budget.** Additional details on these programs are presented in the Research Summary Matrix and the corresponding Research Summary Profiles.

Strongly Supportive Core Research Activities
Advanced Computing and Communications Facility Operations
Applied Mathematics
Atomic, Molecular, and Optical Science
Catalysis and Chemical Transformations
Computer Science to Enable Scientific Computing
Energy Biosciences
Experimental Condensed Matter Physics
Fusion Physics Research on Alcator C-Mod
Fusion Physics Research on DIII-D
Fusion Physics Research on NSTX
General Plasma Science
Geosciences
High Performance Computer Networks
High Throughput DNA Sequencing
Materials Chemistry
Mechanical Systems, Systems Science, and Engineering Analysis
Neutron and Light Sources Facilities
Neutron and X-Ray Scattering
Photochemistry and Radiation Research
Physical Behavior of Materials
Plasma Theory and Computation
Resources and Tools for DNA Sequencing and Sequence Analysis
Scientific Computing Application Testbeds
Separations and Analysis
Structural Biology Research Facilities
Structure of Materials
Theory & Simulations of Matter, Engineering Physics
Understanding and Predicting Protein Structure
Understanding Gene Function

Moderately Supportive Core Research Activities
Advanced Computing Software and Collaboratory Tools
Advanced Fusion Materials Research
Advanced Medical Imaging
Analytical Chemistry Instrumentation
Chemical Energy and Chemical Engineering
Chemical Physics Research
Climate Change Technology Initiative (CCTI)
Engineering Behavior
Environmental and Molecular Sciences Laboratory (EMSL)
Experimental Fusion Physics Support
Experimental Plasma Research (Alternatives)
General Purpose Plant & Equipment (GPP/GPE)
General Technology: Accelerator R&D
Health Risks from Low Dose Exposures
Inertial Fusion Energy Research
Mechanical Behavior and Radiation Effects
Multiprogram Energy Lab Facilities Support (MELFS)
Oak Ridge Landlord
Production DNA Sequencing Facility
Radiopharmaceutical Development
Science Education Support

NOTE: Please see Appendix A for more information on the budgets, the research performers, and other related information for each Core Research Activity.