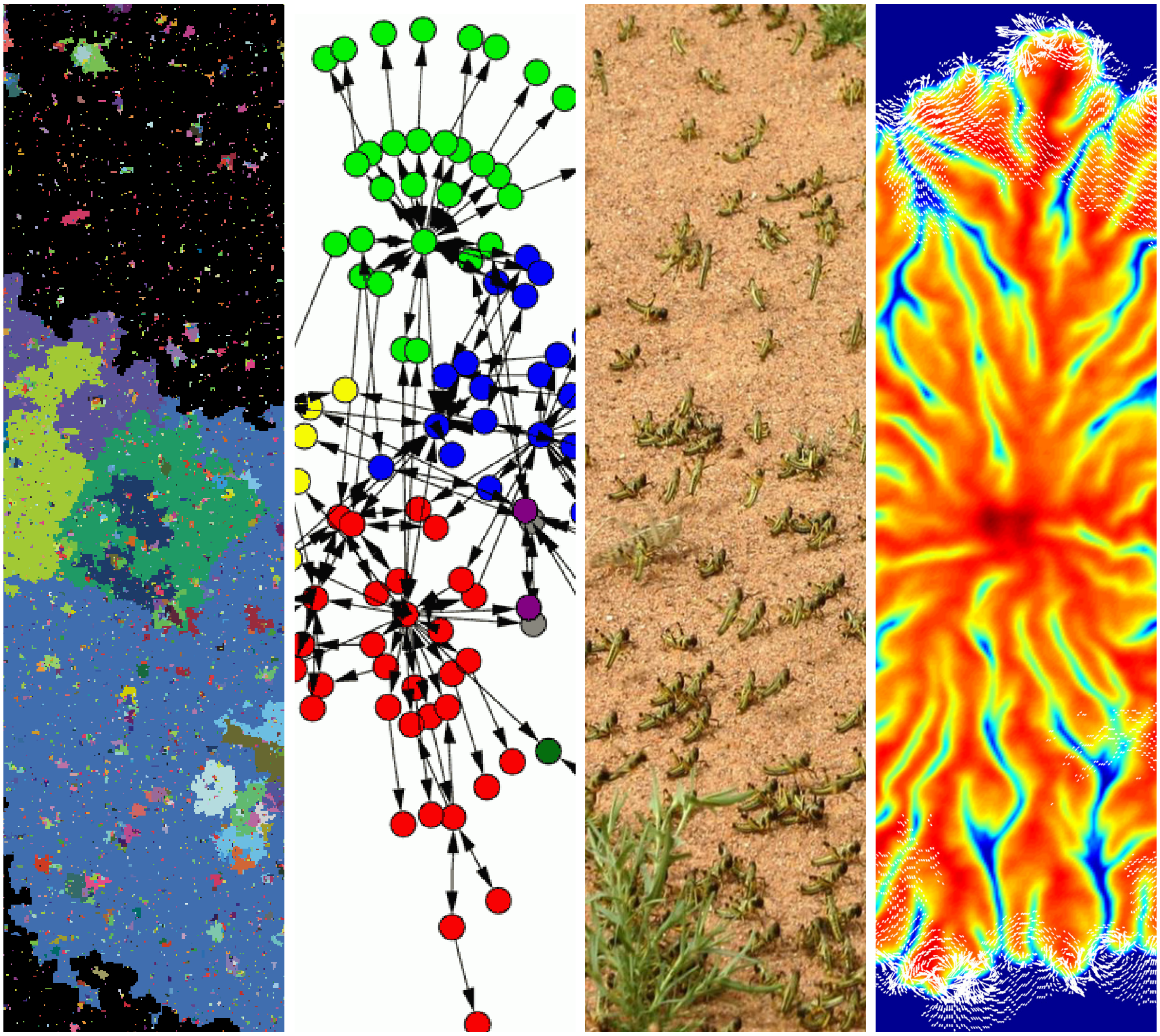

Foundations for Complex Systems Research in the Physical Sciences and Engineering

Report from an NSF Workshop in September 2008

John Guckenheimer, Cornell University, Co-Chair
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Summary

Science and engineering have long sought principles for the organization and understanding of complex systems. The impetus to study complex systems is driven both by

- curiosity as exemplified in the aphorism "*the whole is more than the sum of its parts*" and
- the need to deal with important problems of national interest such as critical infrastructure, sustainability and epidemics .

Many complex systems like the power grid, transportation networks and the web demand immediate attention. They have high levels of uncertainty, lack master plans and are susceptible to breakdowns that could have catastrophic consequences. Stronger foundations for the science of complex systems are needed to mitigate these risks and manage these continually evolving systems. A deeper understanding of complex systems will also facilitate the development of controls and strategies to make systems more efficient.

This report is the outcome of a workshop held at the National Science Foundation September 23-24, 2008. The Engineering and Mathematical and Physical Sciences Directorates charged us to identify "barriers" and "gaps" that impede research on complex systems. Our recommendations are our own and do not signify the endorsement of the National Science Foundation.

The panel found that there are indeed gaps in our understanding of complex systems and our ability to engineer them. Specifically, general principles for engineering and analyzing complex systems are still inadequate to design and operate the complex systems in transportation, communication and power distribution that have become part of our daily lives. They are also insufficient for the scientific understanding of complex natural systems despite our ability to simulate larger and more detailed models. We highlight four questions which seem timely for increased emphasis:

1. *What are the best models for studying complex systems?* Simulations of highly detailed models often fail to explain emergent behaviors. Simpler models can lead to more insight. We lack good methodologies for systematically constructing models on different scales and comparing their properties.
2. *How does the structure of a complex system constrain its emergent behaviors?* When we engineer complex systems, we want to preclude undesirable emergent behaviors and generate or exploit desirable ones. We lack the knowledge to systematically predict these behaviors based upon system structure or design.
3. *What are the consequences of evolution and adaptation in complex systems?* Many complex systems were not created from a single design. Instead they have been built incrementally and modified incrementally to improve their performance. We want to anticipate "tipping points" in which large or abrupt changes in system performance result from small changes in the system.
4. *How do we calibrate complex systems and predict their behavior?* Models of actual complex systems always have large numbers of uncertain parameters. Developing reliable predictions about system behavior in the face of this uncertainty is a major challenge.

1. Introduction:

What is a complex system? Our panel found it more useful to characterize the properties that make a system complex than to draw a boundary between simple and complex systems. Four properties stand out, each of which adds complexity to a system:

1. The system has internal **structure**. This structure may consist of many interacting components, a network that describes which components of a system interact, multiple scales of space and/or time, or symmetry. The components of many complex systems are heterogeneous and form a hierarchy of subsystems.
2. The system has **behaviors** that are not characteristic of those observed in "simple" systems. The term **emergent** is frequently used to describe behaviors that arise from the interaction of subsystems and are not evident from analysis of each subsystem. Chaos in dynamical systems and universality classes of phase transitions are exemplars for the types of qualitative behavior that we would like to understand in complex systems.
3. Systems can adapt to inputs and evolve. **Adaptation** and **evolution** are characteristic of critical infrastructure systems and fundamental to the life sciences.
4. **Uncertainty** is pervasive in complex systems. Quantifying this uncertainty and determining how it propagates throughout the system is a key aspect of reliable prediction and control.

Thus, complex systems can be identified by what they do - display organization without a central organizing principle (emergence) and also by how they may or may not be analyzed - decomposing the system and analyzing subsystems does not necessarily give a clue as to the behavior of the whole.

The study of complex systems runs somewhat contrary to the normal (or reductionist) approach followed in physics and chemistry, for example. The central tenet of these disciplines is that if one understands the elementary building blocks – particles, atoms and molecules – one can formulate problems and infer consequences marching upwards in scales. However, it is clear that this approach, though eminently successful throughout history, has limits. Complex systems, by definition, cannot be understood merely by studying parts in isolation. The very essence of the system lies in the interaction between parts and the overall behavior that emerges from the interactions. The system must be analyzed as a whole.

The charge to our panel was to identify barriers that limit our ability to understand, manipulate, and engineer complex systems. We limited our focus to general, cross-cutting issues that span research on multiple complex systems. This approach draws primarily upon a history of success in statistical physics and dynamical systems theory that have discovered and explained "universal" phenomena that are observed across the sciences and engineering. We seek new concepts and theories that can have a similar impact in the realm of complex systems. One major part of this toolkit, dynamical systems, is well-grounded, and leads to analytical proofs. Others parts of the toolkit, such as agent-based simulations or the emergent body of work known as network theory, are not developed at the same level of rigor. To set the stage for our recommendations, we give several examples that illustrate common themes for research on complex systems – these examples cover a range of science and engineering applications. This is followed by remarks about the history of research on complex systems. We then address our charge directly, describing outstanding issues that we think are critical to complex systems research.

Before doing so it important to make a crucial observation about how our understanding of complex systems fits into the context of engineering. The hallmarks of complex systems are adaptation, self-organization and emergence. No single designer designed the web, the power grid of the US, the air traffic system, the supply chains bringing products from all over the world to the US, or the metabolic processes within a cell. Engineering is, at its very root, about synthesis and consistency: designing and manufacturing things in a particular way. Engineering has typically dealt with complicated systems that have enormous numbers of components, but the system is designed with a detailed plan of how these parts work in unison to accomplish a function. One key defect in a single component can bring the entire system to a halt, so redundancy is built into designs when system failure is not an option. In contrast, complex systems evolve to avoid system failures through adaptation rather than through redundancy.

Complex systems are more uncertain than complicated ones, but we expect their emergent behaviors to be robust to variations of their subsystems. There are many complex systems that engineers have to deal with, even though their overall design has been the result of many disparate actions. There is no option: we cannot rebuild the power grid, supply chains, already constructed buildings, etc. from scratch. We have to deal with them as they are. At the same time, we can learn much about complex systems from the study of organisms and ecological systems that function with high degrees of variation.

The examples in the next section cover a wide range of areas – some are decidedly on the science side, others on the engineering side, and many present aspects of both. In fact, one of the most fascinating aspects of complex systems is the potential for connecting thinking from various disciplines, creating awareness of techniques and problems shared by dissimilar domains, and the potential of generating new cross-boundary ideas.

2. Examples of Complex Systems Problems:

2a. Cascading failures in the power grid

Cascading events such as the spread of failures, congestion, defaults, or disease occur in a variety of complex systems such as power, information, transport, social, and financial networks. These events are often costly but hard to anticipate and avoid. Large blackouts of the high-voltage electrical grid that underpins our nation are a notable example. These blackouts typically have some random initial disturbance followed by a long, complicated series of dependent cascading failures. The failures are dependent because the system is progressively weakened by the failures that have already occurred, making further failures more likely. The August 2003 blackout of 50 million people in Northeastern America started with a few events that cascaded across the northeast. Although such large blackouts are rare, they are sufficiently costly to society that there are strong incentives to prevent them by quantifying and managing their risk.

Cascades range over several scales when a local failure of a single component propagates to a global system failure. Historical data for blackouts for several different countries shows a power law dependence in the distribution of blackout size, indicating that large blackouts are more frequent than might be initially guessed. Moreover, some power system simulations produce cascading failures that show statistical physics features of criticality (power laws, phase transitions) as power system loading is increased. Risk analysis of large cascading blackouts requires both system-level models and detailed models of cascades that are validated with observations. We can seek to exploit universal features of cascading and cross-cutting methods of analysis such as probabilistic branching processes in these investigations. Two goals for this research are to

1. Efficiently estimate model parameters to quantify large blackout risk from a shorter data record of cascades. We cannot wait for decades to quantify large blackout risk by observing their frequency.
2. Explain the observed power laws in blackout sizes and predict their exponents. Socio-technical feedbacks play a role in shaping the long-term power grid reliability: underinvestment in the power grid leads to more blackouts, which in turn leads to more grid investment. Thus there is reason to believe that the network may evolve to display some type of self organized criticality.

The United States will invest substantial amounts of money in its electrical grids and other networked infrastructures in the coming decades. Scientific understanding, analysis and optimization of the complex infrastructure dynamics is a better way to make wise choices than just guessing how these complex systems will behave and placing the nation at risk from either excessive catastrophic failures or investments in unneeded equipment. Another aspect is re-engineering and upgrading the grid to enable comprehensive markets in power, new sources of power, and new loads. Today's system was primarily designed to serve local areas with some backup from neighboring areas and to enable only centralized large power stations and passive consumers. Increased efficiency, flexibility and robustness can be achieved by adopting a complex systems viewpoint: a dynamic global network of supply and demand that will enable many new power sources and loads such as solar and wind, demand response from consumers, electric cars, and trading of electricity in both large and small quantities. This new grid will leverage advances in systems engineering, communications, information technologies, and computer power and will play an essential role in achieving a sustainable, reliable and economic power supply for the nation.

2b. Animal locomotion

The agility, grace and efficiency of animal locomotion are astonishing. Animal locomotion and its control is a complex system: there are complex feedbacks between the nervous and musculo-skeletal systems of the organism. The real time computations done by the nervous system to control locomotion are poorly understood. It hardly seems plausible that humans (or animals) coordinate the large numbers of mechanical degrees of freedom independently while executing tasks like walking, running and swimming. At the same time, we are sensitive to external stimuli and respond to unanticipated inputs as quickly as allowed by the conduction velocities of nerve impulses. We don't understand how these responses are computed by the nervous system. One hypothesis is that control of locomotion utilizes "internal models" with a small number of degrees of freedom and a small number of parameters. In this view, comparison of sensory input with the motion predicted by an internal model provides the information used by the nervous system in controlling locomotion. An extension of this hypothesis is that the control system has been a target of natural selection. Animals may have evolved so that their locomotion is accurately described by their internal models *because* that makes their locomotion easier to control.

One of the challenges in understanding human walking and running is balance. Given that our bodies are similar to an inverted pendulum, how do we remain upright and avoid falling? Indeed, falls are a serious health risk for the elderly. Hierarchies of models are useful to explore this issue. Three types of models for running are

1. a limit cycle of a piecewise smooth dynamical system (an abstract model divorced from physical mechanics),
2. a pogo-stick: a mass on top of a springy leg that bounces on the ground, and
3. detailed biomechanical models of multi-segmented limbs with muscular forces acting at specific attachment points.

These models complement each other and are each useful for different purposes. The abstract models enable us to formulate the problem of stability concisely and to determine dynamical requirements for stability. The pogo-stick has been used as a simple mechanical model to unify data from running in many different animals and to study stability. Analysis of these models explains why some types of perturbations are difficult to stabilize and provides a test bed for the study of control strategies. The detailed models can be compared directly with empirical data, but we lack good methods to systematically estimate all their parameters so that they fit the data or walk stably. Models that incorporate realistic feedback from the nervous system are even more challenging than ones that regard the nervous system as a black box controller.

Research on machine and animal locomotion influence each other. We continue to look at animals for inspiration to build machines that run, fly or swim. At the same time, we can test our theories about the principles underlying animal locomotion by building devices based upon those principles. Most vehicles that we build rely upon different modes of propulsion than animals moving in the same medium, e.g., wheels vs. legs for terrestrial locomotion, thrust from propellers or jet engines instead of flapping for flight. Better methods to engineer systems that rely upon periodic, rhythmic actions rather steady states are needed to build machines that move like animals. Here the complexity that confronts us is agile, real time control of a non-equilibrium system with a large number of degrees of freedom.

On a larger scale, groups of animals form herds, schools and flocks that move in coordinated patterns. We would like to explain how these large scale patterns emerge from interactions among individuals without higher level supervision. We can explore the origin of spatial patterns from specific interaction rules with simulations of agent-based models, but we lack a well developed general framework for carrying out theoretical analysis of how these patterns emerge.

2c. Integrated building design for energy efficiency

Commercial and residential buildings consume significant amounts of energy. In the United States buildings consume 39% of the energy used nationwide and 70% of the electric energy used. Increasing energy efficiency in buildings is a prime target of both the Federal and state strategies for R&D that affect global warming and security as well as industry products that address the increasing impact of fuel prices. “Net zero energy” buildings will require energy efficiency gains over current baselines of roughly 70%, with the remaining savings being provided by renewable energy sources.

Energy is consumed in residential and commercial buildings through a variety of loads. In commercial buildings the highest loads are lighting, heating and cooling. Building subsystems – envelope, thermal, ventilation – strongly interact. A recent report of the American Physical Society (Energy Future: Think Efficiency; http://www.aps.org/energyefficiencyreport/) characterizes the design of energy efficient buildings as a complex system:

> *"A commercial building is a complex system, with the energy use and performance of any one part of the system affecting the energy use of the building as a whole through a complex cascade of interactions. However, the typical design process for commercial buildings is a linear, sequential process that precludes the analysis and design of the buildings as an integrated system. In order to achieve deep savings in energy use, an integrated and iterative design process, involving all members of the design team, is required.*
>
> *Significant interactions among all design elements of a building affect heating and cooling loads (e.g., window size, placement, and thermal characteristics; window shading types and placement; lighting locations, efficacy and local controls; building orientation; number and wattage of plug loads; and the volume of outside air that is circulated into a building).*
>
> *All of these elements need to be considered in light of advanced technology options (e.g., onsite generation, passive ventilation, thermal mass with night ventilation, chilled ceiling displacement ventilation, dehumidification and daylighting). Control strategies and operating conditions for all of the equipment in the building strongly affect the effectiveness of the design and technology choices for the building."*

Current technology is not meeting this challenge. A study conducted by the National Renewable Energy Laboratory (NREL) of six buildings showed that the design goals were not achieved for all six – indeed the design targets were missed by large margins. Subsystems of the buildings are *highly interconnected* and the interconnections that lead in design to energy savings can also lead to higher energy usage due to uncertainties as changes in their interactions are caused by perturbations in construction, the control system operations or weather and occupancy uncertainties. These interactions and the subsequent changes in performance are undesirable *emergent behaviors*.

2d. Parameter estimation for biological networks

The metabolic processes within a cell are a dizzying array of interconnected reactions which may be effectively seen as a network. The removal of a single enzyme from the network—and consequently, its corresponding reaction(s)—can cause the "knockout" of several additional reactions. In each case, the relationship between structure and function is central: How have these systems balanced the need for robustness against perturbations while being adaptable in the presence of dramatic changes? In man-made systems, this balance may be the culmination of concerted human intervention; in natural systems such as metabolic networks, it is the work of evolution. There have been over the last few years several attempts to elucidate the structure of metabolic networks.

Experimental methods like microarrays are used to infer gene regulatory and metabolic networks within cells from correlations in gene expression. Other methods are used to observe protein-protein interactions. Dynamic models can be constructed by viewing the cell as a complex system of chemical reactions and writing differential equations for these reactions. The resulting models are complex and have large numbers of unknown or incompletely known parameters. This uncertainty is typical of complex systems models, especially when it is impossible to isolate the components of a model that contribute to a parameter or to design experiments that measure the parameter directly. Moreover, the parameters may be poorly constrained by the data. This happens when there are "sloppy" directions in the parameter space for which the model behavior is insensitive to changes in parameters along these directions. At the same time, parameter variations that do not lie in these sloppy directions will produce large outputs in model dynamics. As a result, all of the individual parameters have large errors – usually factors of tens to thousands – but certain parameter combinations are well constrained by the data. Nonetheless, falsifiable predictions may be made long before the parameters are remotely known by systematically studying the sensitivity of model output to parameter variations in different directions. It may be possible to characterize the model output in terms of a few parameter directions that are orthogonal to the sloppy directions in the parameter space.

There is recent evidence for universal patterns of sensitivity that express how well a model fits data as its parameters are varied. These sensitivities are measured by eigenvalues that are commonly observed to decrease with uniform ratios: the stiffest eigenvalue is three times larger than the second stiffest, which is three times larger than the next stiffest, and so on. This tantalizing observation suggests strategies for estimating parameters to fit dynamic models to data, independent of the number of parameters. Search algorithms that emphasize parameter variations in the stiff directions result in an enormous gain in efficiency for sampling methods that fit models to data. These methods can also provide a substrate for experimental design in determining which experiments will best help in constraining model parameters further. These issues of parameter estimation are widespread wherever there are models that produce limited ranges of dynamical behaviors but have large numbers of parameters. Many parameter combinations will produce model output which matches the data: only the "stiff" parameter combinations are well constrained buy the data. Thus sloppy model analysis is a tool for quantifying uncertainty and model reduction in complex systems. It systematically identifies manageable numbers of parameters that determine the main features of system behavior.

2e. Soft matter, complex fluids and granular systems

Self-assembly is the term used for the spontaneous organization of (typically soft) matter into structured arrangements. Self-assembly processes are ubiquitous in nature and govern the formation of complex biological structures from viruses to cells. Until recently, much of materials science and soft condensed matter physics involved self-assembly of fundamental building blocks – typically atoms, molecules, macromolecules, and colloidal particles – into bulk thermodynamic phases whose architectures were significantly less sophisticated than those routinely found in nature. However, in the last few years, our ability to fabricate building blocks that can be engineered with great specificity has undergone a quantum leap. We can now synthesize a range of shapes and endow specific areas of these shapes with the desired interparticle forces to drive assembly into complex structures. We are witnessing a revolution in which entirely new classes of particle "supermolecules" can be designed with what can be viewed as programmable instructions for assembly. Advances are occurring at length scales from millimeter-sized plastic wedges that self-assemble when dispersed in water to particles that self-assemble at nanometer scales. These new building blocks are the "atoms" and "molecules" of tomorrow's materials. For example, it is now possible to manufacture colloidal polyhedra, nanocrystals in the form of tetrapods and triangles, and tiny cubes of molecular silica. One emerging approach to confer upon nanoparticles and colloids predetermined "instructions" for assembly is to decorate the surface of the particles with "sticky patches" made from synthetic organic or biological molecules. This strategy is inspired by biology, where the precision of self-assembled structures such as viruses and organelles originates in the selectivity of the interactions between their constituents.

What is possible when traditional molecules are replaced with these new building blocks? What types of ordered structures are possible, and what unique properties could they have? We are just beginning to understand the wealth of possibilities. Theory is providing key insight to guide experiments, but enormous challenges lie ahead in predicting what structures will emerge from a given set of assembling building blocks. Agent-based models, genetic algorithms, and other optimization and simulation approaches from the field of complex systems may provide a powerful complement to more traditional materials simulation methods like molecular dynamics and Monte Carlo simulations. The bridging of techniques from these two fields is fertile ground for studying emergent structures and properties of complex materials systems, especially as these new building blocks grow in complexity,.

Two related areas should be mentioned as well. The first is *dynamic self-assembly*, where particles are self-propelled or otherwise driven and the dissipative motion can produce emergent, persistent patterns far from equilibrium even in the absence of complicated interparticle interactions, for example, spinning magnets on the surface of a liquid that self-organize into complex dynamical patterns in two dimensions. The second area is granular matter, possibly the simplest example of a system where knowing details of the interaction among the elementary building blocks may fail to give a glimpse of the behavior of the global system itself. Some of the most revealing issues are suggested by simple experiments. For example, mixtures of large and small particles in partially filled long rotating cylinders segregate into what appear at the surface to be alternating bands of larger and smaller particles. This happens under a wide range of conditions including mixtures that are wholly immersed in a liquid. Over long time scales the initially segregated structure coarsens with smaller bands forming larger bands. These results do not have a definitive theoretical explanation. Another large area of self-organization of granular matter corresponds to the case of vibrated shallow layers of particles: rod-like grains interacting via excluded volume can form nematic, smectic, tetratic and whirling patterns depending on particle shape and vibration frequency and amplitude.

3. Historical Aspects of Complex Systems Research

The goal of explaining emergent properties in complex systems is not new. A 1948 article by Weaver ("Science and Complexity", *American Scientist* **36**: 536-544) is widely cited as an early call for the study of complex systems. Few tools were available for investigating models prior to the dramatic improvements in computers since that time. Developments in dynamical systems theory during the 1960's and 1970's realized aspects of a general systems theory by providing new concepts and tools for investigating models formulated as systems of ordinary differential equations. Two aspects of this work were remarkable:

1. a deep understanding of chaos (how simple models could produce complex behavior) and bifurcation (how model behavior changes with varying parameters) and
2. surprising theoretical predictions of universal behaviors that were subsequently observed in physical, chemical, engineering and biological systems.

Models were important in this research, but the predictions were typically independent of quantitative details in the models. Indeed, the formulation of good quantitative models remains a challenge for many nonlinear phenomena, especially in the realm of complex systems. The conceptual framework of dynamical systems identifies aspects of system behavior that are determined by the *structure* of the system; e.g., a conservative mechanical system with a particular symmetry group. Mathematical analysis then characterizes the generic properties displayed within classes of systems with similar structure. The resulting theory has surprising explanatory power. It ties together observations of qualitative behaviors in diverse disciplines, serves as a guide to interpreting simulations and provides foundations for algorithms that analyze systems beyond what can be achieved by simulation alone. Statistical mechanics theories of universality classes of phase transitions have a similar character. They too identify specific phenomena that are a consequence of the system structure and apply to all systems which share that structure.

The approaches used in dynamical systems theory and statistical mechanics have had mixed success when used to study complex systems. The issues discussed in the next section of this report pursue this theme, suggesting how these methodologies can be applied more fruitfully in the context of complex systems. In particular, dynamical systems theory and statistical mechanics have progressed through intense investigation of simple models that capture the essence of a general phenomenon. These simple models have frequently arisen within the context of concrete scientific problems. At the inception of this field of research, complex systems researchers chose models like cellular automata that were more abstract. Relating these models to "real world" complex systems has been problematic. Further analysis of proposed models is needed to understand whether and how they explain general phenomena observed in complex systems. Finding the "right" models that explain general phenomena observed in diverse complex systems is one of the problems discussed below as an outstanding research issue.

Insight into common behaviors for complex systems has come from finding models that display particular types of phenomena. Two examples are "power laws" and analysis of graphs and networks. In their simplest form, power laws describe scaling relationships among different variables, such as the length of an organism with its mass, metabolic rate and speed of locomotion. Self similar fractals have non-integer dimensions that are the exponents of power laws. More subtle power laws have been discovered for phase transitions and critical phenomena. As noted above, power laws are associated with higher rates of cascading failures than those predicted by models based upon independent, random events. Research on the statistical properties of networks has grown rapidly during the past decade. The area has had a large impact on a range of other areas, from the understanding of metabolic processes within cells to the spread of ideas within social groups, including online communities brought together by the internet.

4. Issues: Barriers and Gaps:

4a. Modeling:

The largest complex systems issue identified by the workshop participants is modeling:

What are the best models for representing and analyzing the properties of complex systems?

This is a multifaceted question. Viewed on small enough scales, almost any entity appears to be a complex system. Consider a lump of coal. Determining how it fractures when hit with a hammer or how it burns when heated are questions that involve a hierarchy of scales from atoms to centimeters. It may be unrealistic to think that a single model will capture the essence of this complex system. Models that represent the lump as an extremely large collection of interacting atoms in which each atom "decides" what it does based on interactions with its neighbors are prohibitive to simulate. Moreover, the simulation results may be too complicated to yield insight into important aspects of fracture or combustion. Instead, we are likely to want several distinct models for each of the combustion and fracture properties of this system. Useful models usually come from effectively simple descriptions of the system. These models help us to understand, synthesize and predict. If a model is so complex that it exhibits emergent phenomena we do not understand and produces output that is difficult to fit to empirical data, we may get little from the effort required to build and simulate the model. Still, the insight obtained from simpler models may help guide our investigations of more complicated ones. The key issue is how to find and exploit effectively simple descriptions that retain the essential qualitative features of a problem. Models that embody structure that is amenable to mathematical analysis can contribute to significant insight into system behavior, and they can serve as a foundation for the synthesis, operation and control of complex engineered systems.

Models that are "as simple as possible but not simpler" can be systematically derived from a more complex description, invented or hypothesized. *Model reduction* is a term used to describe one of several strategies to systematically derive "effectively simple" models of a complex systems. *Coarse graining* is one of these approaches. Coarse grained models aggregate small components of a system to reduce the number of model components. Detailed information about the multitude of states of the complex system is not retained, yet the most important effects of these details on the system are accurately captured. An example of coarse graining is the derivation of the Navier-Stokes equations of fluid flow from particle descriptions. Analogous methods applied to more complex "multi-physics" systems are a focus of the DOE Applied Mathematics program on Multiscale Mathematics and Optimization. Statistical moment closures and Galerkin approximations of continuum equations are another form of model reduction in which an infinite dimensional model is expanded in terms of modes and then projected onto a space of low order modes. Mathematical tools and procedures for model reduction, from singular perturbations and normal forms to kinetic theory and data-based modeling have a long history of development and success. However, systematic methods of reduction are lacking. Developing generalizations of envelope of equations for systems with a continuum of modes is a long standing problem in this context. Marshaling these techniques in the context of reducing complex systems to simpler ones that are more tractable is a core task for complex systems science and engineering. It is a key enabling technology that mathematical science will provide to complex systems study and engineering.

Normal forms of bifurcations yield a different type of model reduction. Normal forms are low dimensional models that capture the qualitative dynamics of generic bifurcations (in a specified class as described earlier.) The center manifold theorem justifies the reduction of the systems of interest to its normal form in the vicinity of the bifurcation and yields an algorithm for performing the reduction. In the case of higher codimension bifurcations, the theory yields surprising predictions about complicated dynamics that are a byproduct of interactions between modes that become unstable at the same time. On the other hand, normal forms do not provide quantitatively accurate models outside their local domain of validity, so it is useful to embed them in larger models that provide better quantitative agreement with observations.

Analogs of normal forms and the center manifold theorem are lacking for complex systems phenomena. We seek "simple" complex systems that

1. embody phenomena seen within large classes of systems,
2. are amenable to thorough analysis,
3. preserve structure related to the phenomenon of interest and
4. can be systematically mapped back into the more complicated models

It may be unrealistic to think that we can achieve all these goals: instead of a single simpler model that captures the essence of complex system behavior, we may want a hierarchy of models to capture the key behaviors. Identifying the appropriate scales and the units for model components is one of the critical challenges for complex systems research. Formulating a model that is too complicated to analyze or simulate accurately may yield little useful information, but models that are too coarse to produce the behavior of interest are also inadequate. To cite one example, the hope is that we will find models for cascading failures that will help us understand detailed models of the power grid, financial markets, material fracture, the internet, crackling noise of magnetic materials and earthquakes. In some of these cases, simple models have been proposed but their relationship to the complex system is poorly understood from a theoretical perspective. Metrics for comparing the behavior of the simple and complex models are also needed.

Bridging disparate scales in space, time and level of description is a fundamental enabling technology for complex system modeling. While there are many examples demonstrating this, we need to develop systematic frameworks that bring the examples together, fill the gaps between them, and allow us to work with hierarchies of heterogeneous models so that we can get different levels of consistent descriptions across scales. Systematizing methods for model reduction by linking analytical techniques, computational techniques and possibly also machine learning and data mining techniques appears to be a promising research frontier.

4b. From structure to emergent behaviors

For engineering purposes, we need much better tools for predicting emergent behavior of complex systems from their components. An analogy with reaction diffusion systems makes this evident in the design of distributed control systems. Turing demonstrated that diffusion can lead to spatial patterns in a chemically reacting system even when the homogeneous system of reactions has a globally stable equilibrium state. This happens despite the fact that diffusion usually acts to make concentrations more uniform. In the Turing example, different diffusion rates of an activator and inhibitor destabilize a spatially homogeneous equilibrium state. How do we avoid this type of instability that arises from the coupling of large numbers of stable components in systems like the power grid or a commercial building? Preventing such instability is a design goal for many engineered complex systems. Because systems cannot be modeled in full detail, theories that characterize different kinds of instabilities and identify the circumstances in which they occur are extremely useful. For example, bifurcation theory suggests how we can detect an approaching instability in a slowly changing dynamical system. The intellectual terrain of complex systems is varied, leaving us to ask the general question

What is the relationship between the structure of a complex system and its dynamics?

There are many aspects of this question that form whole research areas by themselves. Turing's example is a specific instance of questions about spatial patterns that arise in other settings like fluid dynamics and traffic flow on our highways. Dynamical systems with an underlying network structure are an area of vigorous research activity at this time. Some of the earliest work in this area investigates synchronization. Huygens observed long ago that pendulum clocks hanging from a wall may synchronize with one another due to their weak coupling through vibrations of the wall. In what other circumstances do collections of weakly coupled oscillators synchronize with one another? Theories have been developed for symmetric networks of oscillators. Nonetheless, the question of synchronization remains an important one in pragmatic terms – for example in operating the power grid or a computer.

The relationship between structure and dynamics is of particular interest in the context of networks.

Are there quantities we can measure about the structure of a network that will allow us to make predictions of various features of a dynamical process *on* that network? This problem is a clear bottleneck in current networks research. We have a mountain of data and expertise about structure. We have measures, models, vast data sets, and a well-developed theory of many aspects of network topology. But we have relatively little understanding of dynamical processes on networks. We would very much like to leverage our knowledge of structure to say something about dynamics, but at present, with a few exceptions, we don't know how to do this.

The "blue sky" dream is that, presented with substantial data about the structure of a network and with a definition of the dynamics taking place on it, we could measure some gross summary statistics of the structure and from the results of those measurements make quantitative, if gross, predictions about the dynamics. Examples might include deriving equations of motion for coarse-grained variables, summary statistics for the dynamics, or extreme value statistics. Applications could be widespread. We have data, but little understanding of dynamics, for systems as diverse as the Internet, epidemiological processes, voter models, neural networks, and traffic flow.

The difficulty stems from the lack of developed systematic tools for coarse-graining dynamics on (possibly directed) graphs with very inhomogeneous topologies– substantially fewer success stories exist. Some specific examples where problems of this type were successfully coarse-grained -and the associated tools- include the development of moment closure methods for epidemiological models, and spectral methods for weakly nonlinear problems such as synchronization.

One of the questions about networks that is being studied intensively is how the statistical properties of connectivity in a large network influence the rate at which information (or disease) spreads across the network. We do not know at this time which complex system structures are the important ones for science and engineering, so exploratory research on many possibilities is appropriate. Following Wigner's famous title about the unreasonable effectiveness of mathematics in science, those structures that give rise to extensive mathematical theory may prove to be the most useful.

The role of structure in shaping the dynamics of complex systems is in part an important modeling issue. The example of hybrid dynamical systems illustrates this issue in the context of engineering problems. Hybrid dynamical systems combine continuous and discrete components, possibly in both space and time. There is no standard definition of a hybrid system, and that impedes progress on the topic. A simple example of a hybrid system is a discontinuous vector field that reaches an impasse or deadlock along a boundary. Think of a thermostat that regulates the temperature in a room by turning a fan off or on. At the set point for the thermostat, the room will heat up if the fan is on and will fall if the fan is off. How should the system evolve at the set point? This is a modeling issue, with answers that depend upon the context in which the discontinuous vector field arises. Three sources of an impasse come from (1) reduction of models with multiple time scales to the slow time scale, (2) mechanical systems with impacts and (3) the design of controllers like thermostats or relays that have switches. Each of these settings suggests a different resolution of the impasse, and the dynamics observed in each case is also qualitatively different. Thus the dynamics of a hybrid dynamical system depend upon the structure embodied in the details of how the continuous and discrete time components of the system are modeled. Theory that classifies the different possibilities and characterizes the dynamics of systems that are generic in each context would be very useful in engineering complex systems.

The interplay of theory, experiment and computation will continue to be important for the study of

emergent properties of complex systems. All are needed in the discovery of unifying principles that explain how, where and why emergent properties arise. Empirical data is the beginning and the end: we want to understand and engineer the real world. Simulation is an important tool for detailed study of specific models. With diverse models from the abstract to the highly detailed we can explore the origins and characteristics of emergent properties. Still, many simulation models are sufficiently complex that they are difficult to analyze, so we need theory to provide a guide that helps us interpret and organize simulation results. Theory also directs our attention to interesting phenomena that might otherwise be overlooked, often by highlighting the structural similarities between different systems.
Research programs on complex systems should maintain a balance for the mutual contributions of theory, experiment and computation. Support for the engineering and operation of complex systems that we increasingly rely upon in our daily lives should recognize the value of cross-cutting principles even in work focused upon a particular system.

4c. Evolution and adaptation of complex and engineered systems

Engineering systems evolve in response to society's changing requirements for useful and reliable performance at minimum cost. There are also requirements for adaptability, flexibility, reusability, incrementally improving previous designs and accommodating legacy systems. Engineers continually tinker with systems to improve them, to respond to failures and to meet changing and new requirements. There is an ongoing negotiation among the requirements for performance, cost and risk of failure. Any redesign or upgrade affects how the engineering system is used and this, in turn, affects the requirements. This interaction with and adaptation to the changing environment makes the evolving system complex. If one adds an extra lane to a congested road, no one expects this to necessarily reduce congestion permanently; the traffic flows are not fixed and will adapt to take advantage of the increased capacity.

The nation's power grid is an example of a complex system that evolves continually. It must respond to the challenges of

1. incorporating new, intermittent sources in new locations such as wind and solar,
2. supporting a market in bulk electricity,
3. accommodating new loads such as electric cars and
4. exploiting the ongoing advances in communications, computer power, materials and devices.

Scrapping the trillion dollar grid and redesigning it from scratch is not an option: advances must build on and coexist with components and technologies that are up to 50 years old. Other vital infrastructures such as the internet are similarly evolving. New uses and vulnerabilities of the internet emerge as its performance increases and users and hackers learn new capabilities and encounter new difficulties. Consumer products such as mobile phones and PDAs also evolve interactively with their users. For example, a blackout of Blackberries has immediate implications for upgrading the system so that a similar outage is less likely in the near future. At the same time, new applications on cell phones lead to hackers exploiting the new vulnerabilities. In general, the advances in communications, computing power and cheap sensors allow engineered systems to have new interactions. These interactions present engineering opportunities to increase function, but they also create new vulnerabilities. Just in time manufacturing can save huge amounts of money by reducing inventory, but is more vulnerable to inevitable (and often unforeseen) disruptions. Also, when extreme events such as hurricanes occur, infrastructures can become more strongly linked: an extended loss of electric power will impact cell phones when backup batteries for cell phone towers run out. Loss of cell phones can impede the repair of pumping stations, which in turn allows flooding of backup diesel electric generators in buildings. In 2008, we have seen painful effects of new financial products that allowed credit and default risk to propagate through the economy in new ways. We are living in an increasingly interdependent and linked world relying on networked systems that are themselves more tightly coupled.

The complexity of these systems matters. Changes to a complex system can lead to unexpected effects as the system adjusts or evolves. For example, suppose that system operators of the electrical grid are penalized for shedding load to forestall problems. This will decrease the frequency of small blackouts since shedding load is a small blackout. However, fewer small blackouts will tend to lead to relaxation of operational margins (because of longer intervals where there are no problems) and this makes the system cheaper to operate while increasing the frequency of rare, large blackouts. Similarly, some risk analysts maintain that the increase in safety afforded by airbags is offset by changes in behavior as people drive faster.

More traditional analyses of engineering systems assume a fixed environment that does not interactively evolve with the engineering system itself. In effect, the engineering is considered to be done outside the system itself. Complex systems analysis of the entire evolving and interacting system includes models of the engineering process itself and offers a new perspective that complements and augments traditional approaches. Moreover, the answers obtained by accounting for these complex systems effects can differ from traditional analyses as discussed above. How does the collective dynamics of a large, engineered system change when one has a large number of people interacting with it? One might think that generalizing the system to include the complex dynamics of its evolution could so complicate the analysis as to make it intractable. But complex systems have their own regularities that can be discovered and exploited. For example, the electric power grids show power laws in the distribution of blackout sizes that may arise from the ways that the grid is upgraded in response to blackouts. This evolution of the grid is similar to self-organized criticality in statistical physics. That is, the complex dynamics of power grid evolution can highly constrain the reliability statistics and what is possible in ensuring grid reliability. These complex dynamics may reveal simplicity even as a more complicated context for engineering is represented.

Studying evolved or evolving systems is a new and exciting perspective in engineering. But, of course, it is a foundational perspective in 20th and 21st century biology. As the community probes the engineering of biological networks, there is the potential for exciting interplay between complex systems engineering and the study of biological networks that have evolved such exquisite resilience and adaptability to their environments.

4d. Methods to calibrate, predict and forecast complex systems

Optimally assimilating experimental data into theoretical models for complex systems poses several unusual challenges. Identifying Domain Name System (DNS) Internet attacks, predicting the spread and dynamics of epidemics, estimating probabilities of extreme events, predicting climate and weather, modeling the cell cycle or response of a cell to hormonal stimuli -- all demand the integration of observed behavior into large-scale, multi-parameter models. This problem is addressed in many ways from different disciplines and perspectives. One approach is to cast the problem in a framework that is probabilistic and Bayesian in nature. By viewing the dynamics in light of already available knowledge regarding the events reflected by the data, one can develop hypotheses that form the basis of stochastic (Bayesian) methods.

For models with real-time dynamics and noise, Bayesian methods can be implemented using filtering methods: Kalman filters for linear problems, and more generally optimal nonlinear filtering (NLF) methods. There is a tremendous challenge when taking these ideas to problems involving complex systems due to the computational complexity of nonlinear filters in terms of the dimensionality of the optimization and sampling.

The use of Bayesian methods for fitting multiparameter complex systems models to data poses new challenges and opportunities. Can our theoretical and algorithmic approaches make use of characteristic features that emerge from the conjunction of complex models to the real behavior of complex systems? Can we use these new methods to better forecast/tune/explore/optimize these central issues of social importance?

Indeed, there are surprising, seemingly universal properties that appear to emerge from multi-parameter nonlinear models fit to data, that hint of effective new tools for exploring, fitting, and falsifying these models. The following properties have been observed in a large number of systems biology models, along with models of insect flight, interatomic potentials, high-energy particle accelerators, variational wavefunctions from quantum Monte Carlo, and also from exponential and polynomial fits to data:

(1) Fitting the parameters to match the collective behavior of these models (as opposed to individual measurements of the different parameters) is invariably an ill-posed problem. Indeed, in a typical problem there are only a few directions in parameter space ("stiff" parameter combinations) that are well constrained; many other parameter combinations have thousands of times larger uncertainties. This leads to large error bars, ranging from factors of fifty to thousands, for each of the parameters. Nonetheless, good predictions about subjects of interest appear to be possible. Predicting the result of overexpressing a gene is an "interpolation" between existing experiments, while predicting a binding constant is a wild extrapolation.

(2) This is due to a "skewness" between the parameters chosen to model the system and the combinations of parameters that govern system behavior. Elegant differential geometry approaches (multiparameter theories for manifolds in prediction space) allow us to extend existing algorithms and methods (Jeffrey's prior, Levenberg-Marquardt methods for optimization) with a powerful new perspective, and promise possible breakthroughs for the extremely challenging optimization and sampling problems.

Emergent properties are a common theme in complex systems. Here we find "sloppy model" properties emerge from the modeling process -- seemingly universal shared structures in the covariance matrices and ensembles for complex models from a variety of fields. Optimal experimental design for sloppy models, fast new methods for stochastic Bayesian sampling, new geodesic approaches to assimilating data into complex systems models -- all are emerging from a new, deep understanding of the origins and behavior of these sloppy models.

In complex systems analysis, one often finds a large number of parameters - including initial conditions - whose exact value is unknown. The partial knowledge that we have of such a parameter might be encoded as its probability distribution or as bounds on its maximum and minimal values. In such a situation it is important to understand the sensitivity of the dynamics of the complex system to a range of possible parameter values. In other words, methods for propagation of uncertainty from inputs to the complex system to its outputs are needed. At the present time, even the foundations of the subject of uncertainty propagation - in terms of how uncertainty is measured when it is known as a probability distribution on inputs and propagated through a dynamical system - are poorly studied.

The uncertainty analysis and robust design methods for large nonlinear interconnected dynamical systems are underdeveloped. Prevailing approaches include Monte-Carlo methods, Polynomial Chaos and reliability methods. In these approaches, the structure of the system is not employed, and the system simulation is "brute force." Investment needs to be made into approaches that combine methods from graph theory with dynamical systems and numerical uncertainty propagation methods in order to make progress in designing algorithms that can efficiently propagate uncertainty from inputs to outputs in complex systems.

5. The Next Generation

Education and training of students and postdocs provides both opportunities and challenges in areas of complex systems.

One challenge is bridging the continuum and discrete worlds. Many universities have one course, in many cases several courses, in nonlinear dynamics. This is not the case in agent-based modeling and network theory. However, it can be argued that agent-based modeling, grounded on discrete space and discrete time, is ideally suited to the generation of students that have grown up in a digital world.

Questions involving model development and testing and analysis of data open the door for many opportunities to involve undergraduate students in research. Agent-based models are particularly attractive for undergraduate research problems because the basic models are simple to describe and often yield interesting dynamics from computer simulation. Even more advanced theoretical problems often have a computational component that is suitable for involving undergraduates as part of a research team. They can also be directly involved in data analysis and development of algorithms to work with field or experimental data. At the same time, some of the fundamental theoretical problems proposed in complex systems pose difficult challenges for PhD and postdoc level research, often requiring a multidisciplinary approach or, at the very least, some unification of theoretical ideas from different branches of mathematics and physics. Students may be required to participate in a broader spectrum of courses before they can make significant progress in research, and/or may need to collaborate with other researchers with different expertise in order to solve a problem. Postdocs may find that their PhD research background is missing key components needed to progress in research after the PhD. Therefore, new and creative modes of training of PhD students and postdocs are likely to be necessary in order to make significant further advances in complex systems research. PhD Certificate programs and/or centers in Complex Systems exist at several universities, including Duke, Northwestern University, and the University of Michigan. These provide unique interdisciplinary coursework and seminar opportunities above and beyond the traditional departmental curricula. At the same time, advanced students and postdocs can gain valuable mentoring experience as part of a research team that involves younger graduate students and undergraduates.

6. Recommendation

The National Science Foundation should increase support for research on the fundamental properties of complex systems.

Complex systems appear throughout science and engineering. Mission oriented government agencies pay more attention to complex systems as our social infrastructure becomes more interconnected. However, fragmentation of research funding leaves a void. The benefits of cross-cutting research that reveals common principles of organization of complex systems is manifest. Findings reveal the basis for emergent properties found in seemingly disparate systems and provides the intellectual foundations for engineering the complex systems that are vital in our daily lives. Two aspects of this research are noteworthy:

- The type of research advocated here is complementary to large scale efforts devoted to specific critical infrastructures. This kind of research does not require massively supported large groups: discoveries will result from the efforts of individuals who are empowered to explore models that distill the essence of complex systems in their simplest forms.

- It is crucial, however, to devise mechanisms to foster collaborations among investigators across disciplines. This is important to keep research on these topics well grounded. Multiple perspectives are essential to the solution of complex systems problems.

The National Science Foundation is uniquely positioned to support research with these important characteristics.

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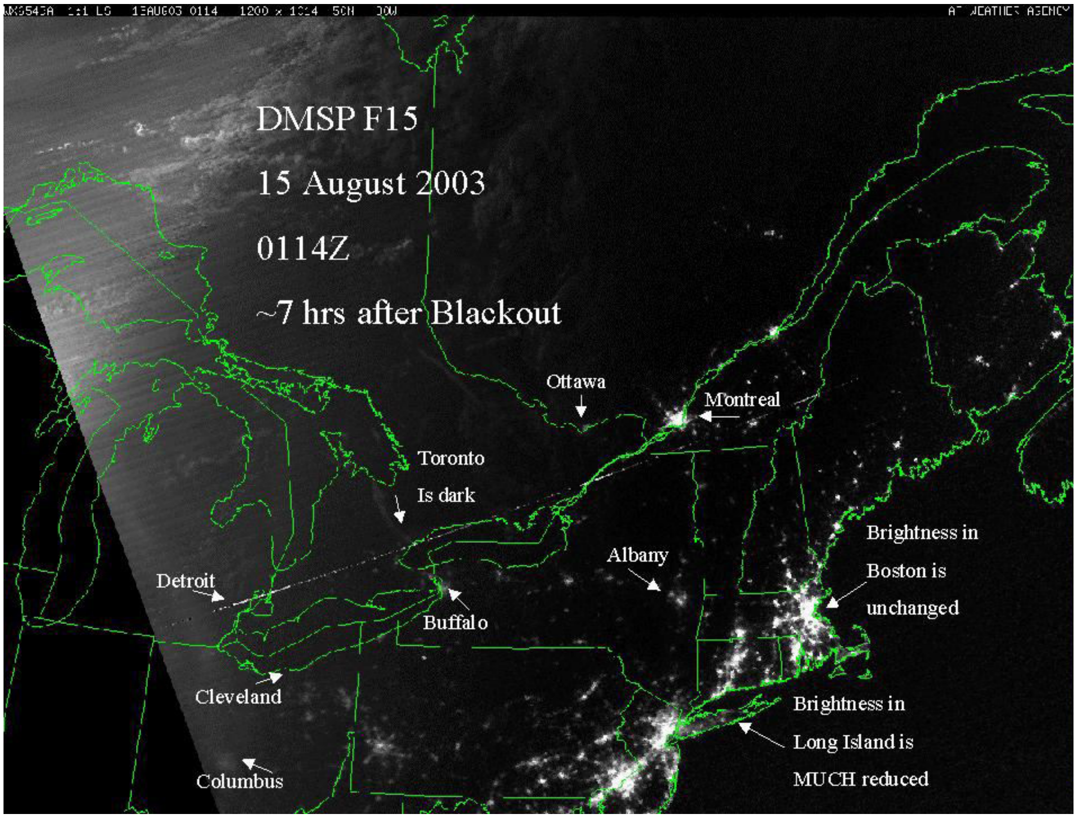

Picture from space of the August 2003 blackout, due to hundreds of cascading failures that started in northern Ohio and propagated to 7 states and 2 provinces. 50 million people lost electrical power and it cost about 8 billion dollars.
Image courtesy of the Air Force Weather Agency

On the cover (from left)

- Cross sections of avalanches in a model of magnetic Barkhausen noise, from James P. Sethna, Karin A. Dahmen, Christopher R. Myers, "Crackling Noise," *Nature* 410, 242 (2001).
- A network representation of pages on a web site. The nodes in this network represent web pages and the connections between them represent hyperlinks connecting one page to another. Reprinted Fig. 13 with permission from M. E. J. Newman and M. Girvan, "Finding and evaluating community structure in networks", *Phys. Rev. E* 69, 026113 (2004). Copyright 2004 by the American Physical Society.
- A 'marching band' of the Desert locust (Schistocerca gregaria). These bands can be tens of kilometers long and have a devastating impact on agriculture. The Desert locust is estimated to affect the livelihood of one in ten people on the planet (photograph by Iain Couzin, Princeton University).
- Numerical simulation of a bacterial colony growing on a wet medium (J. Lega & T. Passot, 2008). Colors represent bacterial density (from low (blue) to high (red)) and the arrows indicate hydrodynamic motions of the mixture of bacteria and water.