Perspective

Complex Systems

J. M. Ottino
Dept. of Chemical Engineering, Northwestern University, Evanston, IL 60208

Introduction

What do metabolic pathways and ecosystems, the Internet, and propagation of HIV infection have in common? Until a few years ago, the answer would have been "very little." The first two examples are biological and shaped by evolution, the third is a human creation, and the fourth is an unwieldy mixture of biology and sociological components. In the past few years, however, the answer has emerged that they all share similar network architectures.

Seemingly out of nowhere, in the span of a few years, network theory has become one of the most visible pieces of the body of knowledge that can be applied to the description, analysis and understanding of complex systems. Several reviews (Strogatz, 2001; Albert and Barabási, 2002) and popular books (Barabási, 2002; Buchanan, 2002) have appeared. At the same time, the release of Stephen Wolfram's controversial book, *A New Kind of Science* (Wolfram, 2002), generated a large number of essays and opinion pieces on the topic of cellular automata and agent-based modeling, although the topic clearly has been around for a while (Tofoli and Margules, 1987; Kauffman, 1993).

By comparison, Chaos Theory—nonlinear dynamics or dynamical systems—seems stately and established, and in fact it is. Nonlinear science and nonlinear dynamics tools are deeply embedded in research and analysis across a wide spectrum of science and engineering. However, the other two components of the triad, agent-based models, and especially network theory, are not part of the standard toolkit of most scientists and engineers.

New results are emerging. Consider three recent examples.

Communication Protocols. Until recently, the models used for developing communication protocols in the Internet were based on random graph models, in which every router has roughly the same number of connections. However, it was shown recently that the real Internet has a scale-free structure, i.e., the distribution of the number of connections decays as a power law (Huberman and Adamic, 1999; Albert et al., 1999; Faloutsos et al., 1999). A few routers have most of the connections. This finding has led to a total redirecting of strategies for developing communication protocols and peer-to-peer search strategies (Adamic et al., 2001; Kleinberg, 2000; Watts et al., 2002). Intriguingly, similar network topologies have been uncovered in the organization of metabolic networks and protein interactions within cells (Jeong et al., 2000; Fell and Wagner, 2000).

Ants and Near-Optimal Paths. Ants have the ability to calculate the shortest path to different food sources using trails of pheromone. Replace sources of foods with cities and ants with salesmen: this analogy leads to a new way to view the classical traveling salesman problem. Ant-inspired simulations developed in the late 1990s have led to algorithms that find near-optimal routes in networks. France Telecom, MCI, and British Telecommunications have used antlike routing strategies to telephone and data networks (Bonabeu et al., 2000).

Thresholdless Epidemics. The classical theory for the emergence of epidemics—based on lattice-like connectivity or random connectivity between individuals—predicts that there is a transmissibility threshold for the onset of an epidemic. Below the threshold, no epidemic can develop; above the threshold, the disease quickly spreads to a steady-state fraction of the population. The actual picture may be much worse. Recent calculations have revealed that infections propagating in a scale-free network have no epidemic threshold, i.e., an epidemic will develop *for all nonzero transmissibility rates* (Pastor-Satorras and Vespignani, 2001). These results, together with the recent discovery that the network of sexual contacts has a scale-free structure, help understand the course of sexually transmitted infections such as HIV (Liljeros et al., 2001). Somewhat unexpectedly, the same theory can explain the spread of virus software through e-mail (Lloyd and May, 2001).

These are exciting results. However, as with everything that appears new it would be incorrect to claim complete novelty. Chaos can be unmistakably traced to Jules Henri Poincaré in the 1890s and networks were studied by mathematicians such as Paul Erdös and Alfréd Rényi in the 1960s, if not earlier. And cellular automata owe their origin to John von Neumann's work in the 1940–1950s. However, what is new is the power of the *entire picture*, not the elements.

This is an appropriate time to pause and survey the landscape. The objective of this article is to present in a unified way recent results in the analysis of complex systems and discuss their impact on chemical engineering. The implications for ChEs are twofold: augmentation of the curriculum and reshaping research—augmentation of what we already do plus access to a whole new array of problems that would have been unthinkable just a few years ago. Chemical engineers, being exposed to a wide range of length scales and trained to think in terms of systems, can seize the opportunity and are perfectly poised to take a leadership position in these exciting new developments.

Complicated and Complex. A discussion about complex systems has to start with the definition and a distinction: what is complex and how does it differ from the merely complicated?

The most elaborate mechanical watches are called *très compliqué*. They are, as their French name implies, complicated. A Star Caliber Patek Phillipe has 10^3 pieces. A Boeing 747-400 has, excluding fasteners, 3×10^6 parts. In complicated systems, parts have to work in unison to accomplish a function. One key defect (in one of the many critical parts) brings the entire system to a halt. This is why redundancy is built into designs when system failure is not an option (e.g., a nuclear submarine).

The stock market, a termite colony, cities, or the human brain are complex. The number of parts, e.g., the number of termites in a colony, is not the critical issue. The key characteristic is *adaptability*. The systems respond to external conditions. A food source is obstructed, and an ant colony finds a way to go around the object; or a few species become extinct and ecosystems adapt.

A word of caution, however. The boundary between "simple" and "complex" is subtle. It takes little for a simple system to become anything but simple. A forced pendulum—with gravity being a periodic function of time—is chaotic. In fact, one can argue that the driven pendulum contains everything that one needs to know about chaos; the entire textbook by Baker and Gollub (1990) is built around this theme. A double pendulum—a pendulum hanging from another pendulum—is also chaotic. And it does not take much to make billiards chaotic. The trajectories of a hard sphere in a circle are regular, but in a stadium—a rectangle with two opposing sides being semicircles—they are fully chaotic (Buminovich, 1974).

Rough Definition of Complex Systems. A complex system is a system with a large number of elements, building blocks or *agents*, capable of exchanging stimuli with one another and with their environment. The interaction between elements may occur only with immediate neighbors or with distant ones; the agents can be all identical or different; they may move in space or occupy fixed positions, and can be in one state or multiple states. The common characteristic of all complex systems is that they *display organization without any external organizing principle being applied*. In the most elaborate examples, the agents can learn from past history and modify their states accordingly. Adaptability and robustness are often the byproduct. Part of the system may be altered, and the system may still be able to function.

Examples of Complex Systems. Complex systems are systems where knowledge of the elementary building blocks—a termite, a neuron—does not even give a glimpse of the behavior of the global system itself, i.e., rich macrodynamical behavior with "simple" elementary building blocks. It is, however, clear that some complex systems are simpler than others. (Semantic difficulties are unavoidable. For example, complexity has a well-defined mathematical meaning in computer science and cryptography, but often multiple ones, often qualitative, in ecology, cognitive science, chemical, physical, and biological sciences.) Possibly, the most unyielding example may be the human brain. At an individual level, we know quite a bit about neurons, but we are nowhere close to comprehending consciousness. The individual elements in food webs or ecosystems are, in a few cases, relatively well understood. This, however, may give no clue as to the robustness and adaptability of the entire system. Possibly, the simplest complex example, one arising in theoretical physics, is the celebrated 2-D Ising model, a caricature of a magnet, a lattice with elements displaying up-down spin behavior. The realm of classical particles or grains and how they interact with each other are well understood. However, how the multitude of length scales that appear in sand dunes—from centimeters to hundreds of meters—arises from the individual particles is far from obvious.

Reductionist Viewpoint. There are three broad categories of complex systems: physical and chemical systems, biological systems, social systems and organizations. It may be argued that physical and chemical systems are the simplest: we know the building blocks. At some level, however, one may argue that everything is a physical and chemical system. And therein lies the paradox. How does complex behavior arise from simple building blocks? Physics is driven by simplicity; the harder one looks, the simpler it gets. But once one reaches the ultimate simplicity (e.g., Newton's laws), how does one manage to put things back together?

The study of complex systems runs somewhat contrary to the normal (or reductionist) approach followed in physics, chemistry, biology, and economics. The central tenet of these disciplines is that if one understands the elementary building blocks—particles, atoms and molecules, a strand of DNA, we can formulate problems and infer consequences marching upward in scales. However, it is clear that this approach, although eminently successful since Galileo's times, has limits. Complex systems cannot be understood 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.

Building Blocks. The concept of building block brings also its own bit of semantic confusion. Quite rightly, many disciplines regard their "elementary building blocks" as *complex*—no one would label a neuron or an individual in an organization as being "simple." Also, it may be difficult to design an experimental methodology, or the key experiments, for studying the elementary block. Or there may be open theoretical questions. Thus, for example, one talks of "complex fluids" in polymer and colloidal science.

In many disciplines, the *systemic* complexity is acknowledged, and the building block is isolated, and analyzed/studied under well-defined conditions. However, these studies often fail to reveal some of the aspects and properties that will allow the conceptual reconstruction of the global system. Consider the case of biology. One of the grand challenges in this area is the *synthesis* of the relevant building blocks (see, for example, p. 85 in Wilson, (1998). Another one is the development of scientific (experimental and theoretical) methodologies for the study of the elementary blocks *in action* as parts of the system they are part of (for example, the attempts to extract evolutionary and functional information from genome sequences, the development of high-throughput techniques, DNA arrays and proteomics, imaging, etc).

Given this avalanche of information, the study of the elementary blocks themselves and interactions between building blocks has become difficult and "complex." In fact, in some areas, biology being the prime example, one could argue that new technologies are providing information at a much faster rate than our ability to digest and understand it. How does our ability to simultaneously monitor and observe complex systems at different scales enhance our understanding of these systems? What are the scientific methods that will allow us to understand these systems (Hatzimanikatis, 2000)?

However, even if the building blocks are "simple," moving upward in scales is far from trivial. Atoms and small molecules are reasonably well understood; the same can be said of colloids and, marching upward, continuum scales. However, the region between 10 and 10,000 Angstroms (1–10^3 nm), the realm of self-assembling molecules, is poorly understood.

There are exciting opportunities, however. An example of exploring "what if" questions is provided by recent work on colloidal systems and "model atoms" (Frenkel, 2002). An especially attractive aspect of colloids is that one has the ability to control the attractive forces between particles by varying solvent, adsorbed molecules, etc. Thus, studying the crystallization of model atoms gives considerable new insight into the role of interobject potentials in self-organization

(Davis et al., 1989). Heuristics are now emerging about manipulation of attractive and repulsive forces to drive colloidal assemblies into desired structures (Pham et al., 2002; Velikov et al., 2002).

Complex Dissipative Systems: Experimental Approaches. Computations provide a route towards understanding. Model experiments provide another. Several recent experimental efforts have focused on the self-organization of systems with designed interplay between attractive and repulsive forces. However, as opposed to the "model atoms" mentioned above, these systems organize, but do so only when they dissipate energy.

One example is a system of magnetic spinning particles maintained at the interface between a liquid and air, or at two close parallel interfaces between air-liquid and liquid-liquid pairs (Grzybowski et al., 2000; Grzybowski and Whitesides, 2002) (Figure 1). Particles spin due to the application of a magnetic rotating field. The confining magnetic field attracts all the particles towards the axis of rotation of the magnet, however, when the particles get close, hydrodynamics forces become repulsive. This results in a competition between the attractive and repulsive effects, and the particles arrange in patterns. Prediction may be nontrivial; it takes just a few classical vortices to produce chaos (Aref, 1983).

Other recent experimental illustrations come from granular dynamics. A classical example is the work of vibrated granular layers of Umbanhowar et al. (1996) (Figure 2). A recent related study, from Arshad Kudrolli's group, which shows how order appears in the most unexpected circumstances, consists of long rods placed in a vibrating container. Depending on the volume fraction above a critical packing fraction, there is formation of dense domains of nearly vertically packed rods that move as large-scale vortices.

Another group of examples entails the competition between chaos (due to mixing) and order (brought up by segregation due to differences in particles' size or density). These may be the simplest experimental examples of systems displaying competition between chaos and order (Hill et al., 1999).

Complex Systems Tools

The mathematical techniques used in complex system studies include nonlinear dynamics, differential and difference equations and time series analysis, cellular automata, graph and network theory, and, depending on the problem, aspects of game theory, Markov processes, information theory, and genetic algorithms. Even a superficial survey is manifestly impossible. We restrict ourselves to nonlinear dynamics, agent-based models and cellular automata, and network theory.

Nonlinear Dynamics and Chaos

Nonlinear dynamics and chaos in deterministic systems are an integral part of science and engineering. The theoretical founda-

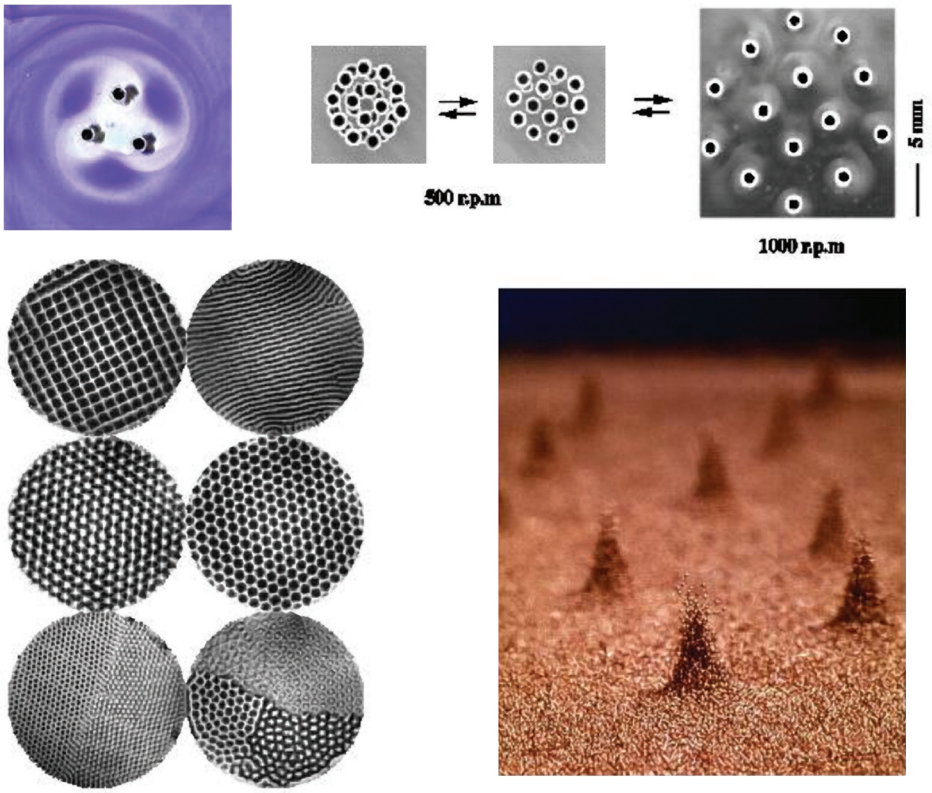

Figure 1. ***Top row*** **(left), millimeter-sized, magnetic disks interacting via vortices generated in the surrounding liquid; (right), at two nearby interfaces, depending on the speed of rotation, crystals form (Grzybowski et al. 2000, Grzybowski, and Whitesides 2002).** ***Bottom row*****, patterns produced by vibrating a thin layer of small brass spheres. Depending on the frequency and amplitude of the oscillations several patterns are possible. The perspective view shows organized "oscillons" (Umbanhowar et al., 1996).**

tions are on firm mathematical footing. There are well agreed-upon mathematical definitions of chaos, many of them formally equivalent. In dissipative systems having an attractor plus one positive Liapunov exponent—a quantification of the divergence of nearby initial conditions—can be taken as a definition of chaos. There are many textbooks—e.g., Baker and Gollub (1990), Strogatz (2000), Ott (1994)—review articles, monographs, and an almost innumerable number of experimental studies, computational applications, and even patents, based on nonlinear analysis tools. There is even the historical perspective provided by massive scholarly studies (e.g., Aubin and Dalmedico, 2002).

There are still, however, many misconceptions about chaos and its implications. Extreme sensitivity to initial conditions does not mean that prediction is impossible. Memory of initial conditions is lost within attractors, but the attractor itself may be extremely robust. In particular, chaotic does not mean unstable.

Chaos means that simple systems are capable of producing complicated outputs. Simple 1-D mappings can do this—the logistic equation being the most celebrated example. In autonomous differential equations a minimum of three dimensions are needed—the Lorenz system being the best known 3-D case. The flip side is that complicated outputs need not to have complicated origins; seemingly random-looking outputs can be due to deterministic causes. Many techniques have been developed to analyze signals and to determine if fluctuations stem from deterministic components. Various techniques, such as multidimensional maps, may reveal characteristic features not observable with conventional data analysis.

Nonlinear dynamics is embedded throughout research; applications arise in virtually all branches of engineering and physics—from quantum physics to celestial mechanics. There are numerous applications in geophysics, physiology and neurophysiology. Even subapplications have developed into full-fledged areas. For example, mixing is one of the most successful areas of applications of nonlinear dynamics (Ottino, 1990); applications to mixing in the ocean constitute a large subarea with entire books and reviews devoted to the subject and the inevitable tendency toward the very specific (e.g., Waseda et al., 2002). Within chemical engineering successful applications have included mixing, dynamics of reactions, fluidized beds, pulsed combustors, and bubble columns. It is clear that nonlinear dynamics does not exist in isolation, but it is now a platform competency. This does not mean that all theoretical questions have been answered and that all ideas are uncontroversial. For example, there is significant discussion about the presence of chaos in physics and the role it may play in determining the universe's "arrow of time," the irreversible flow from the past to the future.

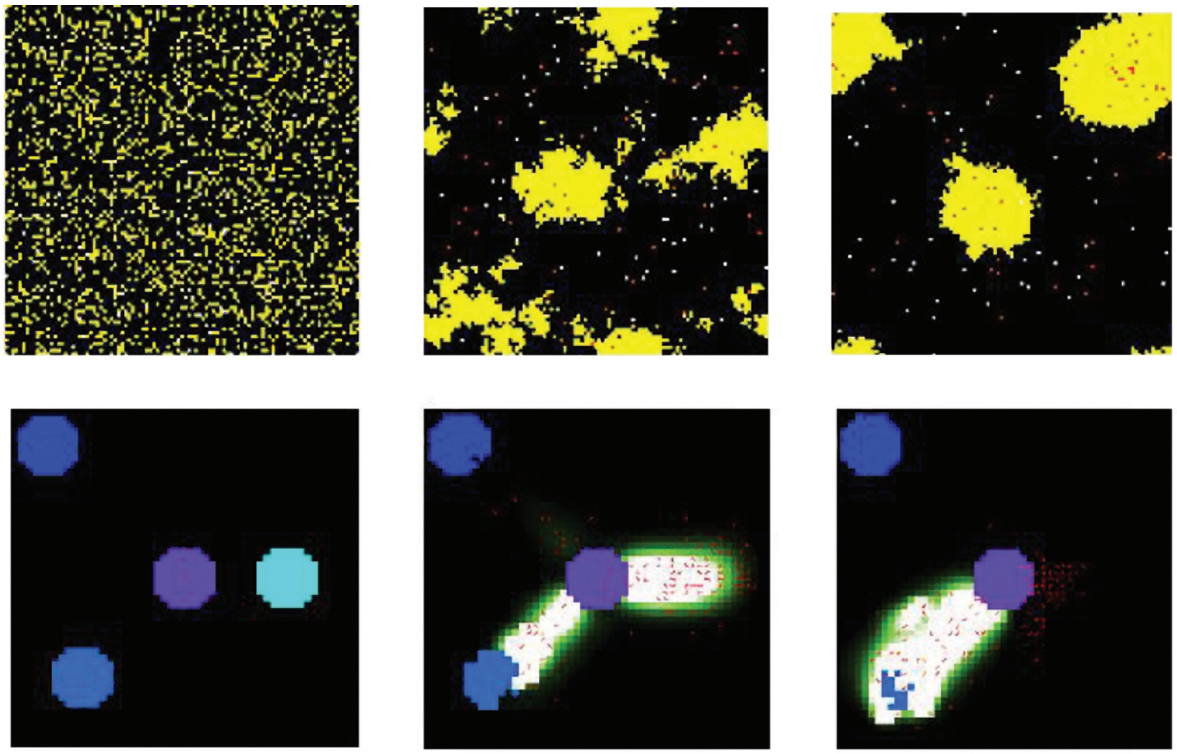

Figure 2. Agent-based models.
Leftmost column shows the initial state; the two other columns show intermediates times, with time increasing left to right. *Top row*, termites build mounds with no central controlling authority. The algorithm is remarkably simple: each termite walks randomly. If it bumps into a wood chip, it picks the chip up, and continues to wander randomly. When it bumps into another wood chip, it finds a nearby empty space and puts its wood chip down. *Bottom row*, ants looking for food (a central nest and three sources of food). Ants move randomly and when they find food go back to the nest depositing a trail of pheromone. Ants tend to follow concentrated paths of pheromone, and as more ants carry food to the nest, they reinforce the chemical trail. In general the ant colony exploits the food sources in order, starting with the food closest to the nest. Both systems can be viewed in ccl.northwestern.edu/netlogo.

Agent-Based Models

Agent-based modeling is based on the assumption that some phenomena can and should be modeled directly in terms of computer programs (algorithms), rather than in terms of equations. Examples arise in physical, chemical, biological and social sciences; they can be as simple as propagation of fire and simple predator-prey models between a handful of species and as complex as the evolution of artificial societies. The central idea is to have agents that interact with one another according to prescribed rules. This type of modeling has started to compete and, in many cases, replace equation-based approaches in disciplines such as ecology, traffic optimization, supply networks, and behavior-based economics.

The origins of agent-based modeling can be traced to *cellular automata*—rows in a checkerboard that evolve into the next row based on simple rules. A physical example may be the propagation of fire in a forest. The trees may be represented as occupying a fraction of the squares in a checkerboard; the rule may be that fire propagates if two trees are adjacent via the face of a square. Thus, fire propagates though faces—up, left, and right, but not diagonally. More generally, the basic building blocks may be identical or may differ in important characteristics; moreover, these characteristics may change over time, as the agents adapt to their environment and learn from their experiences resulting in feedback (see, for example, Epstein and Axtell, 1996). A very large number of didactic and exploratory agent-based models arising in various disciplines appear in Wilenesky (1999).

Consider, for example, a model of social segregation inspired by the work of Thomas Schelling (1978). The reader will note a similarity to the Ising model and spinodal decomposition. This model mimics the behavior of two types of individuals, reds and greens, in a city, which is represented as a checkerboard. The number of reds and greens are equal and empty spaces may be present. Reds and greens get along with each other. However, reds and greens want to live near at least *some* people of their own color. Initially, reds and greens are randomly distributed throughout the city. But many individuals are unhappy, since they do not have enough neighbors with the same color. Unhappy individuals move to new locations, tipping the balance of the local population, prompting others to leave. If red people move into an area, local green people might leave, and *vice-versa*. Over time, the number of unhappy individuals decreases. Simulations show how individual preferences propagate through the city, leading to large-scale patterns, with large clusters of red-green. For example, in the case where each individual wants at least 30% of neighbors with the same color, we end up (on average) 70% same-color neighbors. Thus, relatively weak individual preferences can lead to significant overall segregation. "The interplay of individual choices…is a complex system with collective results that bear no close relation to the individual intent," Schelling wrote.

Some of the most challenging cases of agent-based models may be those involving economics (e.g., Epstein and Axtell, 1996). These approaches differ significantly from classical modeling systems via mathematical analysis. Classical microeconomic analysis assumes that consumers are identical and that they never change their preferences or characteristics; also, the consumers either do not communicate at all or they interact in some type of random fashion. Any inclusion of heterogeneity, organization, or adaptation would require the use of computer simulation or of numerical analysis. Applications of cellular automata to problems familiar to ChEs are those involving fluid flow and flow of granular matter (e.g., Peng and Herrmann, 1995, 1994; Désérable, 2002). These techniques should be considered complementary rather than competitive to continuum-based and discrete-particle methods.

The idea of cellular automatons can be traced to John von Neumann and Stanislaw Ulam, further developed and popularized in Conway's Game of Life, and more recently Wolfram. It is interesting to note that Watson and Crick's work unraveling the structure of DNA took place nearly concurrently with much of von Neumann's study of machine reproduction. It is noteworthy that the logical basis of reproduction in living cells mimics von Neumann's machine reproduction theory; in fact, biology's terminology closely follows von Neumann theory. But the converse is also true. Biology has been instrumental in driving agent-based models. The most celebrated examples are based on the behavior of ants. In fact, ants have become the workhorse of agent-based modeling (see Figure 2).

Ants have the ability to find the shortest path to food sources without using any visual cues. This much is known: Ants deposit pheromones while walking and ants prefer to follow directions rich in pheromone. Also, pheromone diffuses and evaporates, that is, trails do not last forever. These facts explain how ants can find the shortest path if a trail is broken and an obstacle disrupts the trail. The ants that pick the shorter path around the obstacle reconnect more quickly to the interrupted pheromone trail than those that choose the longer path. The pheromone scent is stronger in the shortest path; it gets picked, and over time reinforced. Thus, finding the shortest path around the obstacle *emerges* as a property of the interaction between the obstacle shape and the ants' distributed behavior. The same mechanisms help ants to pick the closest source of foods (Figure 2).

Can ants be used in practical situations? The answer is yes. Consider the traveling salesman problem. Say, for example, that salesmen have to visit ten cities, and that takes different times to travel between any two of them. What is the shortest path where each city is visited once? Consider now that an army of virtual salesmen (ants) are released to explore, randomly, all possible routes in the map. After an ant successfully completes the trip, it traces back the path to the original city, depositing an amount of virtual pheromone along the path. After the first round of explorers, a new batch is released and instructed in some way to follow the most concentrated routes. Because of diffusion and evaporation, the concentration is lower on longer paths. With tens of thousands of ants exploring the map and seeking high concentration routes, short routes accumulate higher concentrations, while long and convoluted routes accumulate almost no pheromone at all. The process is autocatalytic. After several repetitions, the shorter routes are reinforced reaching a near-optimal path. This is precisely the Swarm Intelligence approach devised by Marco Dorigo (see Bonabeau et al., 2000). The method leads to solutions that appear to be better than the Shortest Path routine used by the Internet to find paths between nodes of the network.

Networks

Many systems can be seen as networks: a system of nodes with connecting links. Individuals exchanging e-mails is one example. Person A sends an e-mail to B; if B replies, A and B are connected. Other clear-cut examples are the Internet: how servers are connected, and the World Wide Web, how Web pages are linked. Examples in the biological sciences are food webs and the metabolic and protein networks within cells. In food webs, species are connected if one preys on another; in metabolic and chemical reaction networks, two molecules are connected if they participate in the same reaction.

There are two extreme classes of networks: regular, as in a lattice, where every node connects with the same number of neighbors, and random, where every node has the same probability of being connected to any other node. Consider a few definitions that are used to describe networks. The minimum number of links that must be traversed to travel from node i to node j is called the shortest path length or distance between i and j. A graph is connected if any node can be reached from any other node; otherwise the graph is disconnected. The average *path length* is the average of the minimum number of steps necessary to connect any two nodes in a connected network. The *degree of clustering* is (roughly) the number of actual links in a local subnetwork divided by the number of possible links, i.e., if all sites were connected. Person A is a good friend with both B and C. There is a good chance B and C are also friends. If that is the case, there is local clustering (Albert and Barabási, 2002). The *degree distribution* $P(k)$ is the probability density function of the number of links k of all the sites in a network. In a lattice $P(k)$ is a delta function; in a random network $P(k)$ is a Poisson distribution.

Real networks, however, are not well described by either model (see examples in Figure 3). Real networks are both clustered (high degree of local connectivity) and small (it takes only a small number of steps to connect any two nodes). Real networks appear to be bracketed between two extremes: Egalitarian networks and aristocratic or scale-free networks.

An egalitarian network is a lattice with a few long distance connections randomly thrown in and a few links cut out (Watts and Strogatz, 1998). Adding connections reduces clustering algebraically, but decreases the path length logarithmically; $P(k)$ remains approximately a Poisson distribution. However, the network becomes both clustered and small. These kinds of networks are often referred to as small-world networks. The neural network of the worm *Caenorhabditis elegans*, the power grid of the western U. S., and the collaboration graph of film actors are small-world networks (Watts and Strogatz, 1998; Strogatz, 2001). A surprising recent result is that the onset of small-world phenomena becomes more and more certain as the system size increases (Barthélémy and Amaral, 1999). This has important consequences in social networks. At the local level, all the agents may believe they are interacting in a large-world environment, but in reality they are in a small world, implying that the propagation of information, diseases and technologies is much faster than one would expect for a large world.

In a scale-free network, on the other hand, the number of links per node $P(k)$ follows a power law, with the number of links having k links given by $P(k) \sim k^{-\gamma}$, where γ is positive. Therefore, there is no characteristic number of links per node and the network is scale-free. Examples of aristocratic networks are the metabolic and protein network of various organisms, the Internet and the World Wide

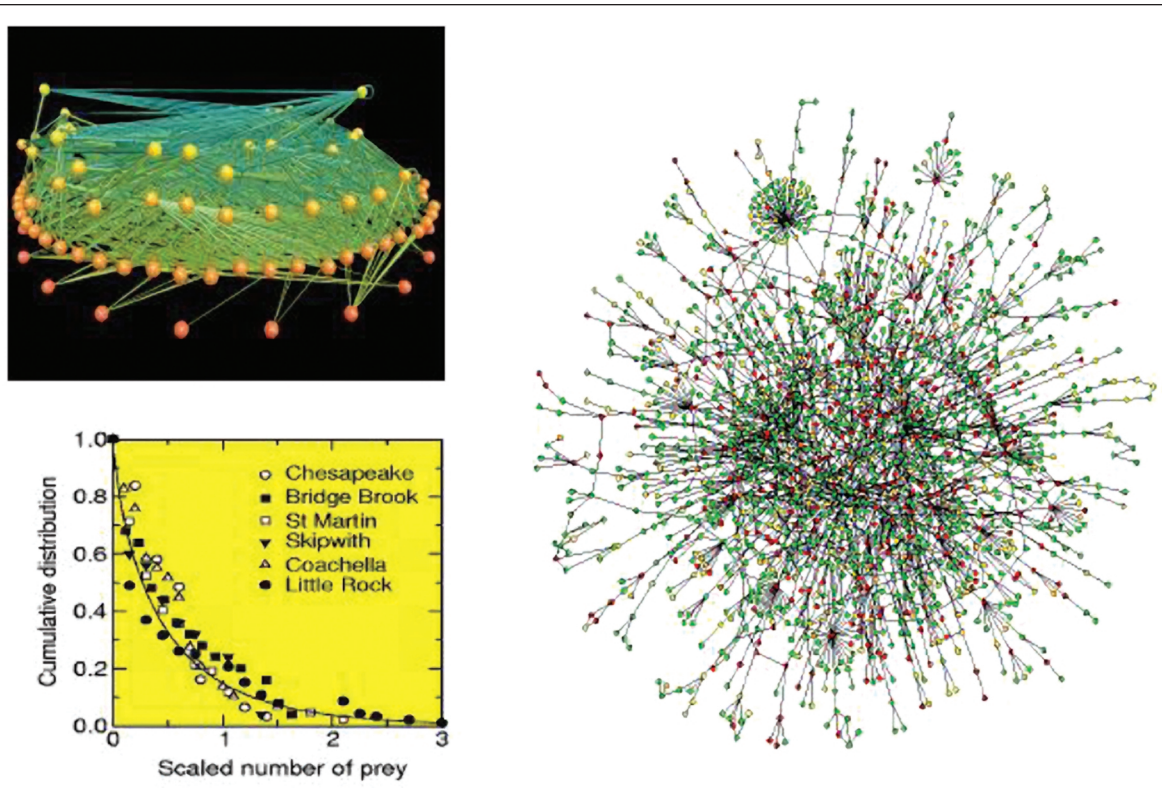

Figure 3. Top left: one of the largest ecosystems ever studied, the food web of Little Rock Lake in Wisconsin. Nodes are species; links connect predators and prey. Height indicates the trophic level; phytoplanktom at bottom, fishes at top. Cannibalism is represented as self-loops (Martinez, 1991 and Williams and Martinez, 2000; courtesy of N. Martinez). Bottom left: Several diverse ecosystems when viewed as networks and plotted in scaled form, show remarkable similarities (from Camacho et al. 2002). Right: Map of protein-protein interactions of the yeast proteome (from Jeong et al. 2001; courtesy of A.-L. Barabási).

Web. The tail of $P(k)$ decreases less rapidly than in a Gaussian; $\exp(-k^2)$ goes faster to zero than $k^{-\gamma}$ does. The "fat tail" property allows for the possibility of highly connected nodes, such as the home page of CNN or Google or, in a more ChE-relevant example, the adenosine triphosphate (ATP) in a cell's metabolic pathway.

There are two aspects to networks, one is the topology or architecture; another is the process that generates the network itself. The architecture alone provides powerful insights. For example the presence of scale-free topology has implications for the robustness of the network, i.e., the ability of a network to function in spite of failures and/or concerted attacks, and even our ability to understand the functional role of genes in model organisms. For example, early analytic studies based on random graph theory suggested that food webs become more fragile as they get large. Recent studies suggest the opposite: the larger the network, the more robust it is.

There is an important downside to the scale free topology though: In a random graph an infectious disease dies once the probability of infection falls below a threshold (the probability of A infecting B falls below p); however, there is no threshold in a power-law network (Pastor-Satorras and Vespignani, 2001). On the other hand, the very structure of the network suggests the mode of treatment: Drugs are most effective in curtailing the epidemic if administered to the people with the most connections.

What are the dynamics of network formation? The scale-free structure of networks can be explained, at least in part, in terms of preferential attachment (Barabási and Albert, 2001; Newman, 2001); in many instances there are significant advantages in connecting to the most connected sites (the Web being one example). On the other hand there may be costs and other physical constraints. An example arises in air traffic. The more flights connect to hubs, say Dallas or Chicago, the more unmanageable hubs become. Preferential attachment reaches a limit (Amaral et al., 2000).

There have been several studies searching for simple generic laws governing the formation of networks. There is some evidence for the existence of universal mechanisms controlling the emergence of universal network structures in ecosystems (Camacho et al., 2002) (Figure 3). This may be an appropriate point to refer the reader to the examples mentioned at the very beginning of this article.

It is a truism that everything is connected to everything else. It is clear that in a system as complicated as the biosphere we have no way to predict the outcome of our actions. Many environmental policies are based more on conviction than on hard science. Network theory is providing the first glimpse to rationally comprehend the dynamics of these processes. This presents enormous opportunities for our profession. Studies of complex reaction networks (e.g., Gleiss et al., 2001) should be part of standard chemical engineering.

Perspectives—Futures Uses

The study of complex systems grew along many seemingly independent strands and, as with nearly anything that is new, it grew in a disorganized way. Also, as with many such interdisciplinary developments, the central ideas spurred analogies in places far away from their initial conception. The danger, however, is that ideas may be stretched beyond their original validity. Science is littered with claims that turn out to be too optimistic. And invariably too much optimism generates proportional negative reactions. Witness the 1995 *Scientific American* article, "From Complexity to Perplexity" (Horgan, 1995). It is important to recognize also that often the claims do not originate in the science and engineering community. Consider the confluence of nanotechnology, biotech, and agent-based swarm intelligence in Chrichton's new novel, *Prey*.

But much has happened since 1995. This much is clear: Many important problems cannot be decomposed; looking at subparts does not provide the answer and they must be looked at as a whole. The elements described above provide some of the tools. However, much remains unexplored; deviations will be discovered and surprises will be unveiled. For example, Willinger et al. (2002) argue that the scale free interconnection structure of the Internet cannot be wholly explained in terms of preferential attachment. This is to be expected: it is obviously easier to find deviations from a model than to identify classes of models that explain many observations. But simply seeking deviations without seeking generality is pointless. One should focus on what has been accomplished and use this as a launching pad to generate further understanding. There is a very practical side to this search. Many problems are being examined now that no one would have thought possible just a few years ago. However, one should recognize that the understanding generated is of a different kind. The equations of a good theory or a good model can be used to make testable predictions based on controlled experiments in the lab. In some of the systems mentioned here—say the examples of ecosystems—conventional lab experiments are not possible. Thus, understanding what this area means and how it can be exploited requires a broader outlook and a change of perspective. Consider the case of metabolic networks. The problem is not finding the data. What network analysis has revealed in this case is structure that otherwise would have remained hidden (Fell and Wagner, 2000). One may not be used to the idea that revealing structure it is the result. However, this fact alone opens a number of questions and avenues of inquiry that otherwise would never have occurred, even shedding light on evolution itself.

It is clear that these tools can and should be taught. Many universities have one course, in many cases several, in nonlinear dynamics. This is not the case in agent-based modeling and network theory. Social sciences and economics are more advanced than engineering in this regard. 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. The many examples in *ccl.northwestern.edu/netlogo* are suited for academic instruction, and agent-based modeling tools are being developed in many institutions (Wilensky, 1999, 2003; Wilensky and Reisman, 1998). But there is little activity on the networks side.

Problems where chemical engineers can have a significant influence are:

- Design of self-organizing materials and self-organizing systems; directed self-assembly; use of fields to govern self-organization, modeling in terms of agent-based algorithms.
- Modeling of fluid flows and flow and segregation in granular matter.
- Modeling of gene and protein interaction-networks, immunology.
- Complex reactions, network analysis of the fate of pollutants, leading to science-based environmental policies.
- Understanding of product and manufacturing supply chains. Supply chains in economics.
- Studies of complex fluctuations in physiologic systems including the ability of systems to respond to multiple environmental stimuli.
- Design of safety critical systems; analysis of failures in distributed systems
- Study of propagation of epidemics.

• Understanding and evolution of organizations, including the design of structures for scientific and technological collaboration.

The above listing is undoubtedly incomplete. It is apparent that chemical engineers, if they seize the opportunity and embrace the study of complex systems and associated techniques, can significantly augment the intellectual basis of the discipline and expand considerably the boundaries of chemical engineering research.

Acknowledgments

I would like to thank Luis Amaral, Bartosz Grzybowski, Vassily Hatzimanikatis, Paul Umbanhowar, and Uri Wilensky for comments during the preparation of this article and providing figures, and to Neo Martinez and Albert-László Barabási for providing material for Figure 3.

Literature Cited

Adamic, L. A., R. M. Lukose, A. R. Puniyani, and B. A. Huberman, "Search in Power-Law Networks," *Phys. Rev. E*, **64**, 046135 (2001).
Albert, R., and A.-L. Barabási, "Statistical Mechanics of Complex Networks," *Rev. of Modern Physics*, **74**, 47 (2002).
Albert, R., H. Jeong, and A.-L. Barabási, "Diameter of the World Wide Web," *Nature*, **401**, 130 (1999).
Amaral, L. A. N., A. Scala, M. Barthélémy, and H. E. Stanley, "Classes of Small-World Networks," *Proc. Nat. Ac. Sci USA*, **97**, 11149 (2000).
Aref, H., "Integrable, Chaotic, and Turbulent Vortex Motion in Two-Dimensional Flows," *Ann. Rev. of Fluid Mech.*, **15**, 345 (1983).
Aubin, D., and A. D. Dalmedico, "Writing the History of Dynamical Systems and Chaos: Longue Durée and Revolution, Disciplines and Cultures," *Historia Mathematica*, **29**, 273 (2002).
Baker, G. L., and J. P. Gollub, *Chaotic Dynamics: An Introduction*, Cambridge University Press, Cambridge, U.K. (1990)
Barabási, A.-L., and R. Albert, "Emergence of Scaling in Random Networks," *Science*, **286**, 509 (2001).
Barabási, A.-L., *Linked: The New Science of Networks*, Perseus Publishing, Cambridge (2002).
Barthélémy, M., and L. A. N. Amaral, "Small-World Networks: Evidence for a Crossover Picture," *Phys. Rev. Lett.*, **82**, 3180 (1999).
Bonabeau, E., M. Dorigo, and G. Theraulz, "Inspiration for Optimization from Social Insect Behaviour," *Nature*, **406**, 39 (2000)
Buchanan, M., *Nexus: Small Worlds and the Groundbreaking Science of Networks*, Norton, New York (2002).
Buminovich, L. A., "On Ergodic Properties of Some Billiards," *Funct. Anal. Appl.*, **8**, 254, (1974).
Camacho, J., R. Guimerà, and L. A. N. Amaral, "Robust Patterns in Food Web Structure," *Phys. Rev. Lett.*, **88**, 228102 (2002).
Davis, K. E., W. B. Russel, and W. J. Glantsching, "Disorder-to-order Transition in Settling Suspensions of Colloidal Silica—X-ray Measurements," *Science*, **245**, 507 (1989).
Désérable, D., "A Versatile Two-Dimensional Cellular Automata Network for Granular Flow," *SIAM J. Appl. Math.*, **62**, 1414 (2002).
Epstein, J. M,. and R. L. Axtell, *Growing Artificial Societies: Social Science from the Bottom Up*, Brookings/MIT Press, Cambridge, MA (1996).
Faloutsos, M., P. Faloutsos, and Ch. Faloutsos, "On Power-law Relationships of the Internet Topology," *ACM SIGCOMM'99*, 251 (1999).
Fell, D. A., and A. Wagner, "The Small World of Metabolism," *Nature Biotechnology*, **18**, 1121 (2000).
Frenkel, D., "Playing Tricks with Designer 'Atoms'," *Science*, **298**, 65 (2002)
Gleiss, P. M., P. F. Stadler, and A. Wagner, "Relevant Cycles in Chemical Reaction Networks," *Adv. Complex Systems*, **1**, 1 (2001).
Grzybowski, B. A., and G. M. Whitesides, "Three-Dimensional Dynamic Self-Assembly of Spinning Magnetic Disks: Vortex Crystals," *J. Phys. Chem. B*, **106**(6), 1188 (2002).
Grzybowski, B. A., H. A. Stone, and G. M. Whitesides, "Dynamic Self-Assembly of Magnetized, Millimeter-Sized Objects Rotating at a Liquid-Air Interface," *Nature*, **405**, 1033 (2000).
Hatzimanikatis, V,. "Bioinformatics and Functional Genomics: Challenges and Opportunities," *AIChE J.*, **46**, 2340 (2000).
Hill, K. M., D. V. Khakhar, J. F. Gilchrist, J. J. McCarthy, and J. M. Ottino, "Segregation-Driven Organization in Chaotic Granular Flows," *Proc. of National Acad. of Sci.*, **96**, 11701 (1999)
Horgan, J., "From Complexity to Perplexity," *Scientific American*, 74 (June, 1995).
Huberman, B. A., and L. A. Adamic, "Internet-Growth Dynamics of the World-Wide Web," *Nature*, **401**, 131 (1999).
Jeong, H., B. Tombor, R. Albert, Z. N. Oltvai, and A. L. Barabási, "The Large-Scale Organization of Metabolic Networks," *Nature*, **407**, 651 (2000).
Jeong, H., S. P. Mason, A.-L. Barabási, and Z. N. Oltvai, "Lethality and Centrality in Protein Networks," *Nature*, **411**, 41 (2001).
Kauffman, S. A., *The Origins of Order: Self-Organization and Selection in Evolution*, Oxford University Press, Oxford (1993).
Kleinberg, J. M., "Navigation in a Small World—It Is Easier to Find Short Chains Between Points in Some Networks than Others," *Nature*, **406**, 845 (2000).
Liljeros, F., C. Edling, L. A. N. Amaral, H. Stanley, and Y. Aberg, "The Web of Human Sexual Contacts," *Nature*, **411**, 907 (2001).
Lloyd, A. L., and May, R. M., "Epidemiology—How Viruses Spread Among Computers and People," *Science*, **292**, 1316 (2001).
Martinez, N. D., "Artifacts or Attributes? Effects of Resolution on the Little Rock Lake Food Web," *Ecological Monographs*, **61**, 367 (1991).
Newman, M., "Clustering and Preferential Attachment in Networks," *Phys. Rev. E*, **64**, 25102 (2001).
Ott, E., *Chaos in Dynamical Systems*, Cambridge University Press Cambridge, U.K. (1994)
Ottino, J. M., *The Kinematics of Mixing: Stretching, Chaos and Transport*, Cambridge University Press, Cambridge, U.K. (1990)
Pastor-Satorras, R., and A. Vespignani, "Epidemic Spreading in Scale-Free Networks," *Phys. Rev. Lett.*, **86**, 3200 (2001).
Peng, G., and Herrmann, H. J., "Density Waves and 1/f Density Fluctuations in Granular Flow," *Phys. Rev. E*, **51**, 1745 (1995).
Peng, G., and Herrmann, H. J., "Density Waves of Granular Flow in a Pipe Using Lattice-Gas Automata," *Phys. Rev. E*, **49**, R1796 (1994).
Pham, K. N., A. M. Puertas, J. Bergenholtz, S. U. Egelhaaaf, A, Moussaïd, P. N. Pusey, A. B. Schofield, M. E. Cates, M. Fuchs, and W. C. K. Poon, "Multiple Glassy States in a Simple Model System," *Science*, **296**, 104 (2002).
Schelling, T., *From Micromotives to Macrobehavior*, Norton, New York (1978).
Strogatz, S. H., *Nonlinear Dynamics and Chaos*, Westview Press, Cambridge, U.K. (2000).
Strogatz, S. H., "Exploring Complex Networks," *Nature*, **410**, 268 (2001).
Tofoli, T., and N. Margules, *Cellular Automata Machines: A New Environment for Modelling*, MIT Press, Cambridge, MA (1987).
Umbanhowar, P. B., F. Melo, and H. L. Swinney, "Localized Excitations in a Vertically Vibrated Granular Layer," *Nature*, **382**, 793 (1996).
Velikov, K. P., C. G. Christova, R. P. A. Dullens, and A. van Blaaderen, "Layer-by-Layer Growth of Binary Colloidal Crystals," *Science*, **296**, 106 (2002).
Waseda T., and H. Mitsudera, "Chaotic Advection of the Shallow Kuroshio Coastal Waters," *J. Oceanography*, **58**, 627 (2002)
Watts, D. J., and S. H. Strogatz, "Collective Dynamics of 'Small-World' Networks," *Nature*, **393**, 440 (1998).
Watts, D. J., P. S. Dodds, and M. E. J. Newman, "Identity and Search in Social Networks," *Science*, **296**, 1302 (2002)
Wilensky, U., *NetLogo. (ccl.northwestern.edu/netlogo)*, Center for Connected Learning and Computer Based Modeling, Northwestern University (1999).
Wilensky, U., "Statistical Mechanics for Secondary School: The GasLab Multi-agent Modeling Toolkit," *Int. J. of Comput. for Mathematical Learning*, Special Issue on agent-based modeling, in press (2003).
Wilensky, U., and K. Reisman, "ConnectedScience: Learning Biology through Constructing and Testing Computational Theories—A Multi-agent Modeling Approach," *Int. J. of Complex Systems*, **234**, 1 (1998).
Williams, R. J., and N. D. Martinez, "Simple Rules Yield Complex Food Webs," **404**, 180 (2000)
Willinger, W., R. Govindan, S. Jamin, V. Paxon, and S. Shenker, *Proc. Nat. Acad. Sci. USA*, **99** (supl1), 2573 (2002).
Wilson, E. O., *Consilence*, Knopf, New York (1998).
Wolfram, S., *A New Kind of Science*, Wolfram Media, Champaign, IL (2002).