Spontaneous Order, Evolution, and Life

Complex dynamical systems can sometimes go spontaneously from randomness to order; is this a driving force in evolution?

HAVE WE MISSED SOMETHING about evolution—some key principle that has shaped the development of life in ways quite different from natural selection, genetic drift, and all the other mechanisms biologists have evoked over the years?

Among the 300 physicists, computer scientists, and biologists who gathered in Santa Fe recently for the second workshop on artificial life,* there seemed little doubt that the answer is "Yes!" And the missing element, they say, is spontaneous self-organization: the tendency of complex dynamical systems to fall into an ordered state without any selection pressure whatsoever. Examples quoted at the workshop include the origin of life itself, which may have happened as simple molecules organized themselves into a kind of primitive metabolism; the self-regulation of the genome to produce well-defined cell types; and even the postulated sudden waves of evolutionary change known as "punctuated equilibrium."

Advocates of spontaneous organization are quick to admit that they aren't basing their advocacy on empirical data and laboratory experiments, but on abstract mathematics and novel computer models. Indeed, as Scripps Institute biochemist Gerald Joyce points out, "They have a long way to go to persuade mainstream biologists of the relevance [of this work]."

Speaking as a mainstream biologist himself, however, Joyce also says he is reasonably sympathetic. At its best, he says, the kind of mathematical and computational models being talked about at the artificial life workshop could give experimental biologists a fresh and coherent framework for understanding all the data they're getting.

No one at the workshop was a more articulate proponent of that view than University of Pennsylvania biochemist Stuart A. Kauffman, who has been a pioneer in theoretical biology for more than two decades.

Ever since Darwin, says Kauffman, organisms have been seen as ad hoc contraptions, the result of random mutations followed by natural selection. "But Darwin didn't know about self-organization," he says. Basically, the theory of spontaneous self-organization was developed starting in the 1960s to resolve a long-standing paradox. On the one hand there is the physicists' Second Law of Thermodynamics, which can be roughly paraphrased as "you can't unscramble an egg"; atoms and molecules are always doing their best to randomize themselves into a state of maximum disorder. But on the other hand there are snowflakes, organized weather patterns such as hurricanes, recurrent sunspot cycles on the sun, and a host of other such phenomena: order and organization seem ubiquitous in nature despite the second law.

* Artificial Life II, 5 to 9 February 1990, Santa Fe, New Mexico.

Los Alamos National Laboratories/Santa Fe Institute

Life and "A-Life." *The workshop's poster captured the mood.*

What resolves this paradox, says Kauffman, is the fact that all these ordered systems are taking in energy from the outside. And when that happens, he says, the second law does, in fact, allow ordered structures to form over a local region. Perhaps the simplest example is a simmering pot of soup, where the upward flow of heat from the stovetop causes the liquid to organize itself into a regular pattern of upwelling convection cells.

If this kind of self-organization is also characteristic of living systems, says Kauffman—and there is no reason to think that living organisms are any different from other physical systems in this regard—then evolution is not just a series of accidents. Evolution is a combination of natural selection *and* spontaneous order, interacting in ways that are both profound and still not well understood.

Indeed, he says, biological self-organization may have contributed to the genesis of life itself—a subject taken up in more detail by his collaborator Doyne Farmer, who is a physicist with the Los Alamos National Laboratory and a coorganizer of the artificial life workshop.

Roughly 4 billion years ago, Farmer points out, life managed to bootstrap itself into existence from a soup of amino acids, simple sugars, and such—chemical building blocks that are thought to have formed quite readily on the infant Earth. And yet the odds against these building blocks randomly linking up into the massively complex proteins and nucleic acids of a modern cell seem astronomical, if only because a substantial amount of energy is needed to form the chemical bonds between them. So how *did* it happen?

One possible answer is that the building blocks organized themselves through chemical catalysis. This suggestion actually dates back in various forms about two decades, says Farmer, although no one until recently has been able to do much with it. But starting with a mathematical analysis of the problem by Kauffman in 1986, says Farmer, and continuing with a computer model that he, Kauffman, Norman Packard of the Santa Fe Institute, and Los Alamos' Richard Bagley have developed, it has now become much clearer just how this kind of self-organization could have occurred.

The basic idea starts from the common laboratory observation that a mixture of amino acids and other small compounds *will* occasionally link up by themselves to form short polymeric molecules. Moreover, many of these small polymers have weak catalytic effects on other reactions. So suppose that polymer A can catalyze the formation of another molecule, B. Now suppose that B catalyzes another reaction to produce C and so on, until somewhere down the line there is a molecule Z that catalyzes the creation of A. The result would be a collection of self-reinforcing reactions known as an "autocatalytic set."

Once such a system formed, says Farmer, it would function very much like a primitive metabolism. It would take in a steady supply of energy and "food" in the form of amino acids and other simple chemicals. It would catalyze the conversion of these monomers into its own member species. And it would end up greatly enhancing the concentrations of its member compounds—including some very large polymers that might conceivably be the precursors of modern proteins and other biomolecules. Indeed, says Farmer, the origin of life and the origin of metabolism might very well have been the same event.

The challenge, of course, is to show that autocatalytic sets could have arisen in practice as well as in principle. As a first step, Farmer and his colleagues have used their computer model to study when the autocatalytic sets will and will not form. Essentially the model is just a simplified version of protein or nucleic acid chemistry: all it has are one-dimensional chain molecules such as *acaddbacd*, which react by joining at the ends and splitting apart in the middle, and a steady input of simple "food" molecules such as *a*, *b*, and *aa*. The researchers can then juggle reaction rates, catalytic strengths, and other parameters to see what works.

Intriguingly enough, says Farmer, the sets *do* form—but only if the system has enough diversity. If all the molecules in the set have the same catalytic strength, for example, then the result is a very low concentration of long polymers. But if each species has a different strength, then those long-chain polymers tend to be much more abundant. Equally intriguing is the fact that some sets seem to be very sensitive, collapsing as soon as there is even a minor variation in their food supply. But others seem to survive quite well—and still others respond by growing and becoming more complex.

Growth, diversity, and adaptation to the environment—autocatalytic sets seem to have some remarkably life-like properties, says Farmer. He and his colleagues are beginning to think about applying these lessons to a new round of wet lab experiments, to see if they can make the autocatalytic sets work with real chemistry.

Biological self-organization may help explain not just how life began, but how it evolved into complex organisms consisting of many different types of cells. Kauffman devoted much of his own talk at the workshop to explaining how this process might work.

Every human cell, he points out, contains roughly 100,000 genes, including an unknown number of regulatory genes, all switching each other on and off through an enormously complex network of interactions. Now, this might seem like a recipe for utter chaos, says Kauffman, since you might expect a system this complex to thrash around forever. And yet it doesn't: except

"Darwin didn't know about self-organization" —*Stuart Kauffman*

perhaps in the case of cancer, the genome always organizes itself into stable patterns of activity corresponding to specific cell types—one for a white blood cell, another for a smooth muscle cell, and so on. How?

Biochemists have been trying to explain it by looking at genetic regulation in exquisite biochemical detail, tracing out exactly how specific genes make specific proteins, how those proteins act back on the DNA to influence other genes, and so on. But Kauffman has taken another tack entirely, building a mathematical model that idealizes the genetic regulatory system purely as a network of interactions: gene A turns on gene B; gene B turns on gene C and inhibits gene D, et cetera. The payoff, he says, is a model that illuminates how complex behavior can arise in *any* genetic system, not just the ones that exist in humans or fruit flies.

Perhaps Kauffman's most striking finding is that the formation of stable cell types may not be an evolutionary accident. In his model genomes, explains Kauffman, cell types correspond to stable, self-reinforcing patterns of gene activation known to mathematicians as "attractors." And by using a branch of mathematics known as dynamical systems theory, he has shown that the formation of such a pattern is almost inevitable, no matter how disorganized the network was to start with. The dynamics of gene interaction, in short, seems to force the genome into a form of spontaneous self-organization.

Lending credence to that possibility are a number of quantitative predictions. For example, Kauffman calculates that the number of attractors in a given model genetic system—that is, the number of cell types—should be roughly proportional to the square root of the number of genes it has. And in fact, says Kauffman, the available data suggest that that relation is approximately true over a wide range of real species, from yeasts to humans.

More recently, says Kauffman, he has been using a very similar approach to study the process of coevolution, in which multiple species compete or cooperate with each other within a larger ecosystem. The idea is to represent the interactions between species as interactions between two or more of his model genomes. Think of a tree evolving better and better natural insecticides to protect itself against bark-boring beetles, says Kauffman, while the beetles are developing stronger and stronger immunities: each improvement in the genome of one species forces a change in the genome of the other.

In the computer simulations he has done to date, the model ecosystems do show a number of features that seem strikingly reminiscent of real ecosystems, says Kauffman. For example, the simulations typically contain a number of species that remain "frozen" for quite a long time, in much the same way that sharks and cockroaches have survived with little change for hundreds of millions of years. At the same time, however, the simulations always contain a number of rapidly evolving species engaged in a kind of "evolutionary arms race," rather like the tree and the beetles.

But perhaps the most intriguing aspect of the simulations is the fact that this pattern of change and stasis itself evolves, says Kauffman. In the subtly shifting network of competition and cooperation, predator and prey, a fast-evolving species might suddenly freeze and cease to evolve for a time, while a formerly stable species might suddenly be forced to transform itself into something new. The fossil record of the latter process would then resemble "punctuated equilibrium": a pattern of stasis interrupted by sudden change, which some paleontologists now believe to be the norm in real evolution. Furthermore, says Kauffman, the simulations also show that on very rare occasions, vast avalanches of change will spontaneously sweep through the ecosystem transforming almost everything. The fossil record of such an event would then look very much like the "great extinctions" that are known to have occurred throughout the history of real life on Earth. However, says Kauffman, his model suggests that such extinctions can occur not only because of random asteroid impacts, but simply because of the natural dynamics of species-species interactions.

This same pattern of stasis punctuated by sudden change also showed up in a number of other ecosystem models presented at the workshop, even when those models seemed superficially quite different. Does this mean some more general mechanism is at work, some theory that could account for the behavior of these models—and perhaps real life—no matter how they are structured?

Maybe. Los Alamos computer scientist Christopher Langton, another coorganizer of the workshop, devoted his own talk to an approach that he hopes may lead to exactly such a theory. To begin with, he says, look at the species that are frozen in models such as Kauffman's. Mathematically, such behavior is reminiscent of the rigid way atoms are organized in a crystal. If that were all there was to living systems, says Langton, then they wouldn't be very interesting. The mathematics would describe cells that couldn't differentiate, ecosystems that couldn't adapt to a changing environment, and organisms that couldn't evolve.

At the opposite extreme, says Langton, look at those species involved in constantly shifting evolutionary turmoil. Their behavior is reminiscent of the way molecules are constantly banging around in a gas. This kind of behavior is described by the mathematical theory of chaos, says Langton, and if *that* were all there was to living systems, then they wouldn't be very interesting either. Cells, organisms, and ecosystems would have no structure or stability whatsoever.

However, says Langton, what the models at the workshop seem to suggest is that evolution drives living systems to a critical point halfway between these two extremes, where they can maintain a vital mix of stability *and* change. At that point, he says, the random-seeming avalanches of stasis and change are mathematically similar to what happens in a piece of matter right on the brink of a phase transition, where submicroscopic regions of solid and fluid are constantly forming and dissolving everywhere in the system. Langton calls this hypothetical critical point "the edge of chaos," and suggests that it may be a fundamental characteristic of *any* complex dynamical system, whether it be a piece of matter, a computer, or a living organism.

Through a systematic set of computer simulations he has verified that such a critical point does exist in simple, two-dimensional dynamical systems known as cellular automata. (For computer afficionados perhaps the best known cellular automaton is "The Game of Life," which gives rise to astonishing complex patterns from just a few simple rules, and which turns out to lie very close to the critical point.) Langton is currently trying to understand whether this transition can occur in more general situations.

He is also the first to admit that this idea is still a long way from being a complete theory. Nonetheless, it has an undeniable appeal—if only because of the irresistible way he describes it: "Life," says Langton, "exists at the edge of chaos."

■ M. Mitchell Waldrop

The Chase Continues for Metallic Hydrogen

In pursuit of a strange beast found only at extremely high pressures, researchers disagree about whether it has been spotted

In theory, it's a simple experiment. Just squeeze a sample of hydrogen gas between the two faces of a diamond press. At about 57,000 times normal atmospheric pressure the hydrogen turns solid. Keep squeezing. At some point well over a million atmospheres, a dramatic change will occur. The hydrogen, originally an insulator, suddenly becomes a conductor—metallic hydrogen. It's a far cry from the usual image of hydrogen as the lightest and least substantial of all the elements, and theorists have predicted a number of strange properties for it. Metallic hydrogen might be a room-temperature superconductor, for instance, or it could be a liquid at absolute zero.

That's the theory. Unfortunately, the practice is not nearly so simple. In addition to the technical difficulties of squeezing a sample with millions of atmospheres, researchers have found it tricky to determine exactly what it is they are producing in the tiny space between the two diamonds. With no chance to touch the sample directly, they must rely on measurements made through the diamonds, which themselves are affected by the intense pressures.

Despite these obstacles, there have been at least two recent reports from teams that think they may have seen hydrogen turn metallic. In the 23 June issue of *Science*, Ho-Kwang "Dave" Mao and Russell Hemley at the Carnegie Institution of Washington wrote that above 2 million atmospheres hydrogen starts to become opaque, a good sign of the transition to a metal. And at a meeting* of the American Physical Society last month, Isaac Silvera claimed that his team at Harvard University has solid evidence that one special form of metallic hydrogen appears at 1.5 million atmospheres.

However, the difficulties with interpreting these experiments remain so huge that scientists are arguing among themselves about exactly what they have pressured hydrogen into doing. At the APS meeting, for example, some scientists said they found Silvera's evidence far from convincing. On the other hand, the Carnegie Institution team claimed the Silvera result is nothing new. They spotted the transition to a metallic state last year, they said.

These arguments aren't mere arcana. If one could make metallic hydrogen, astronomers could study a material that may make up large parts of Jupiter and other superheavy planets. Fusion scientists see metallic hydrogen as a possible fuel—if a stable form exists, as some theories predict, it could be made at several million atmospheres and then handled at normal pressures, providing a nearly ideal fuel for reactors. And condensed matter physicists would love to study what is likely to be a structurally simple yet exceedingly strange material. What could be stranger than the same element that lifted zeppelins over the ocean turning out to be a superconductor at room temperature or a liquid at absolute zero?

So plenty of scientists are waiting to see just how closely reality matches up with the current theory. In essence, theorists calculate that it should take somewhere between 2.5 million and 4 million atmospheres to make "atomic metallic hydrogen," the form of hydrogen that is predicted to be a room-temperature superconductor. Such high pressures would cause the hydrogen molecules to dissociate into pairs of single atoms. But it may not be necessary to squeeze quite so hard to get metallic hydrogen. According to some calculations, "molecular metallic hydrogen" should form at a significantly lower pressure—somewhere between 1.7 million and 2.5 million atmospheres. In this case, the molecules would remain intact.

Carnegie's Mao and Hemley have attempted to test these predictions by taking hydrogen to over 3 million atmospheres. Their report in *Science* last year of hydrogen's opacity above 2 million atmospheres indicated that some of the electrons attached to the hydrogen molecules move into new energy levels and become conduction electrons at these pressures. The existence of conduction electrons would make the hydrogen sample a metal, or at least a "semimetal," Mao said at the time.

Now Silvera says he has evidence that hydrogen becomes metallic at only 1.5 million atmospheres, significantly lower than predicted. At this pressure, the hydrogen sample shifts its structure into what Silvera

*The 1990 March meeting of the American Physical Society, 12 to 16 March, Anaheim, California.